ACCESS DB # 217344

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Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: MARK BERCH Examiner #: 59193 Date: 3/6/07

Art Unit: 1624 Phone Number: 2-0663 Serial Number: 10511537

Location (Bldg/Room#): 5C01 (Mailbox #): 5C18 Results Format Preferred (circle): (PAPER) DISK

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: _____

Inventors (please provide full names): _____

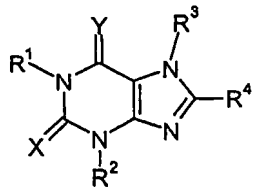
03-298

Earliest Priority Date: _____

Search Topic:

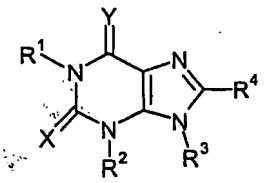
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*



(Ia)

or



(Ib)

wherein:

one of X and Y represents S, and the other represents O or S;

R^1 represents hydrogen or C1 to 6 alkyl;

R_3, R_4, R^2 = H | C(L1)(L2)(L3) chain — must have only single bonds attached

L_1, L_2, L_3 = H | C | O

20070312-10511537-str.rtf

****

STAFF USE ONLY

Searcher: MSB

Searcher Phone #: 1

Searcher Location: _____

Date Searcher Picked Up: _____

Date Completed: 3-12-07

Searcher Prep & Review Time: 60

Online Time: 67

Type of Search

_____ NA Sequence (#)

_____ AA Sequence (#)

2 Structure (#)

_____ Bibliographic

_____ Litigation

_____ Fulltext

_____ Other

Vendors and cost where applicable

1030 STN _____ Dialog

_____ Questel/Orbit _____ Lexis/Nexis

_____ Westlaw _____ WWW/Internet

____ In-house sequence systems

____ Commercial ____ Oligomer ____ Score/Length

____ Interference ____ SPDI ____ Encode/Transl

_____ Other (specify)

INVENTOR SEARCH

=> fil capl; d ibib ed abs hitstr
FILE 'CAPLUS' ENTERED AT 12:31:52 ON 12 MAR 2007

FILE COVERS 1907 - 12 Mar 2007 VOL 146 ISS 12
FILE LAST UPDATED: 11 Mar 2007 (20070311/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

Search #1

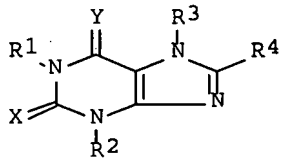
L20 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:855927 CAPLUS Full-text
DOCUMENT NUMBER: 139:350580
TITLE: Preparation of xanthinethione derivatives as myeloperoxidase inhibitors
INVENTOR(S): Hanson, Sverker; Nordvall, Gunnar; Tiden, Anna-Karin
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003089430	A1	20031030	WO 2003-SE617	20030415
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2480452	A1	20031030	CA 2003-2480452	20030415
AU 2003224548	A1	20031103	AU 2003-224548	20030415
EP 1499613	A1	20050126	EP 2003-721211	20030415

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

BR 2003009012	A	20050201	BR 2003-9012		20030415
CN 1646531	A	20050727	CN 2003-808355		20030415
JP 2005526836	T	20050908	JP 2003-586151		20030415
NZ 535406	A	20060831	NZ 2003-535406		20030415
ZA 2004007815	A	20051004	ZA 2004-7815		20040928
US 2005234036	A1	20051020	US 2004-511537		20041015 <--
NO 2004004998	A	20050118	NO 2004-4998		20041117
PRIORITY APPLN. INFO.:			SE 2002-1193	A	20020419
			SE 2002-2239	A	20020717
			WO 2003-SE617	W	20030415

OTHER SOURCE(S): MARPAT 139:350580
ED Entered STN: 31 Oct 2003
GI



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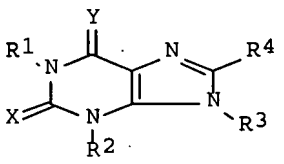


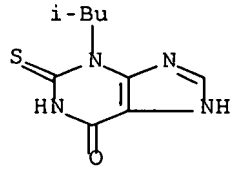
II

AB Xanthinethiones I and II [one of X and Y = S, the other = O, S; R1, R3, R4 = H, alkyl; R2 = H, (un)substituted alkyl] were prepared for use as myeloperoxidase (MPO) inhibitors in the treatment of neuroinflammatory disorders. Thus, Me2CHCH2NHCSNH2 was cyclized with NCCH2CO2Et to give 6-amino-1-isobutyl-2-thioxo-2,3-dihydro-1H-pyrimidin-4-one which was nitrosated, reduced to the 5,6-diamine, and cyclized with HCO2H to give II [R1, R3, R4 = H, R2 = CH2CHMe2, X = S, Y = O]. This compound had IC50 for inhibition of MPO of 0.87 μM.

IT **618913-16-9P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of xanthinethione derivs. as myeloperoxidase inhibitors)

RN 618913-16-9 CAPLUS

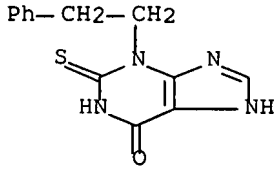
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(2-methylpropyl)-2-thioxo- (9CI) (CA INDEX NAME)



IT **139460-82-5P 618913-20-5P 618913-24-9P**
618913-25-0P 618913-26-1P 618913-27-2P
618913-28-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of xanthinethione derivs. as myeloperoxidase inhibitors)

RN 139460-82-5 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(2-phenylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



RN 618913-20-5 CAPLUS
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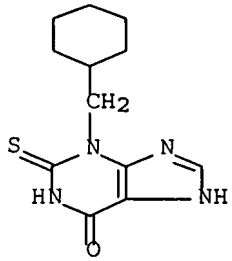
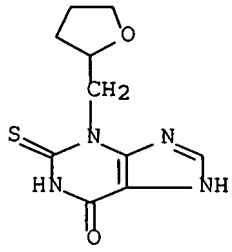
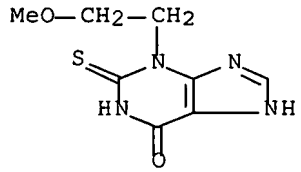


RN 618913-24-9 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[(tetrahydro-2-furanyl)methyl]-2-thioxo- (9CI) (CA INDEX NAME)



RN 618913-25-0 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(2-methoxyethyl)-2-thioxo- (9CI) (CA INDEX NAME)



RN 618913-26-1 CAPLUS
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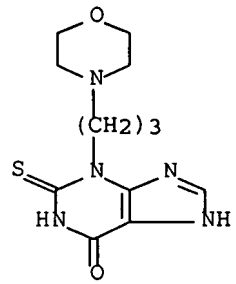

RN 618913-27-2 CAPLUS
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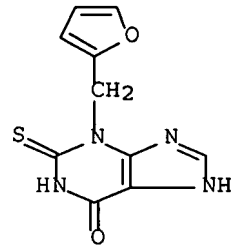

RN 618913-28-3 CAPLUS
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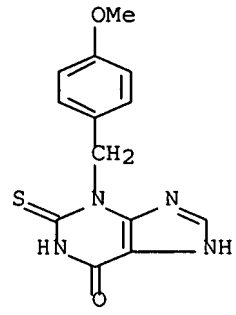
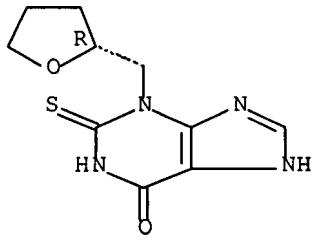


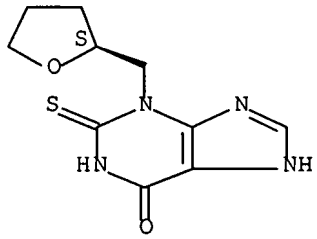
IT **618913-30-7P 618913-31-8P**
RL: PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of xanthinethione derivs. as myeloperoxidase inhibitors)
RN 618913-30-7 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[[(2R)-tetrahydro-2-furanyl]methyl]-2-thioxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

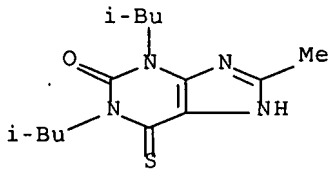


RN 618913-31-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[[(2S)-tetrahydro-2-furanyl]methyl]-2-thioxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **618913-11-4P 618913-12-5P 618913-13-6P**
618913-14-7P 618913-15-8P 618913-17-0P
618913-18-1P 618913-21-6P 618913-22-7P
618913-23-8P 618913-29-4P 618913-32-9P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of xanthinethione derivs. as myeloperoxidase inhibitors)
RN 618913-11-4 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-methyl-1,3-bis(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



RN 618913-12-5 CAPLUS
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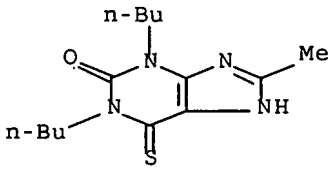

RN 618913-13-6 CAPLUS
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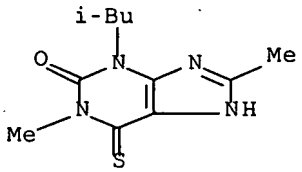

RN 618913-14-7 CAPLUS
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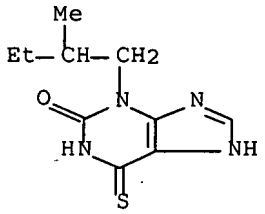

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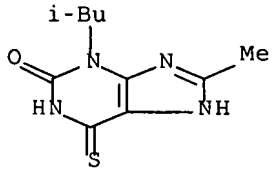

RN 618913-17-0 CAPLUS
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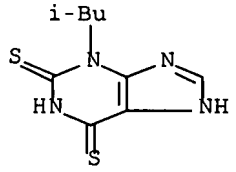

RN 618913-18-1 CAPLUS
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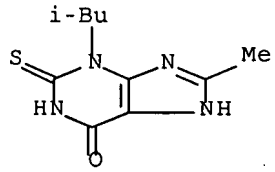

RN 618913-21-6 CAPLUS
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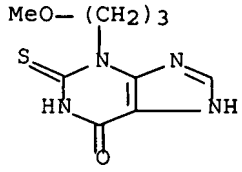

RN 618913-22-7 CAPLUS
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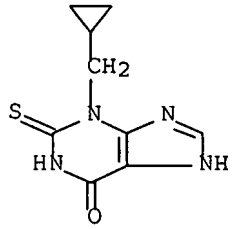
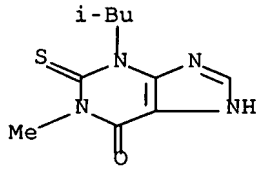


RN 618913-23-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-3-(2-methylpropyl)-2-thioxo- (9CI) (CA INDEX NAME)



RN 618913-29-4 CAPLUS
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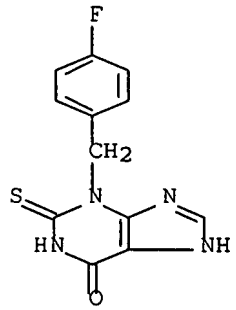

RN 618913-32-9 CAPLUS
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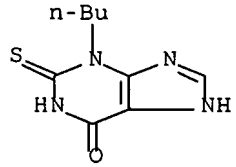


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

STRUCTURE SEARCH

=> fil reg; d stat que l7
FILE 'REGISTRY' ENTERED AT 14:42:39 ON 12 MAR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 MAR 2007 HIGHEST RN 926007-42-3
DICTIONARY FILE UPDATES: 11 MAR 2007 HIGHEST RN 926007-42-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

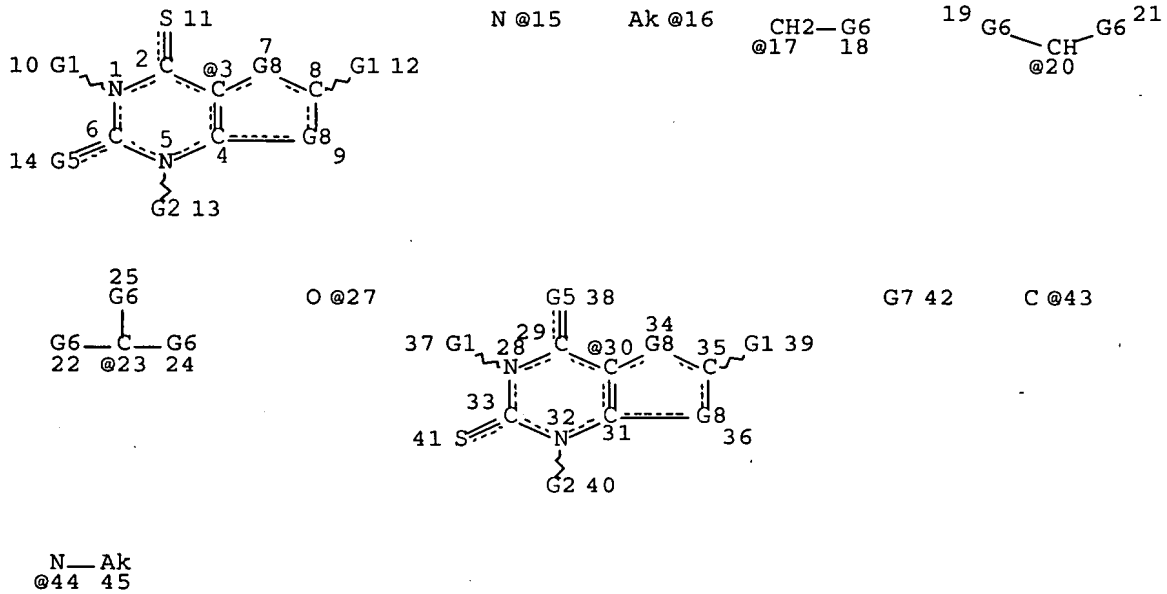
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

L4 STR



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VAR G2=H/ME/17/20/23
VAR G5=O/S
VAR G6=27/43
VAR G7=3/30
VAR G8=15/NH/44
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NSPEC   IS RC     AT  43
CONNECT IS X3  RC AT   8
CONNECT IS E2  RC AT  15
CONNECT IS E1  RC AT  16
CONNECT IS X3  RC AT  35
CONNECT IS E1  RC AT  45
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  44

STEREO ATTRIBUTES: NONE
L7          242 SEA FILE=REGISTRY SSS FUL L4


=> =>
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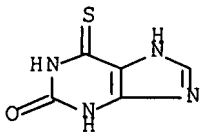
3 REGISTRY NUMBERS YIELDED ~200 REFERENCES.
ONLY THE OLDEST 5 PATENTS FOR EACH PROVIDED HERE.

=> d ide l10

L10 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN **2002-59-7** REGISTRY
ED Entered STN: 16 Nov 1984
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo- (9CI)
CN Xanthine, 6-thio- (6CI, 7CI, 8CI)
OTHER NAMES:
CN 2-Hydroxy-6-mercaptopurine
CN 2-Hydroxy-6-thiopurine
CN 3,6-Dihydro-6-thioxo-9H-purine-2(1H)-one
CN 6-Mercaptoxanthine
CN 6-Thioxanthine
CN NSC 12160
DR 3782-88-5
MF C5 H4 N4 O S
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CSCHEM, DDFU, DRUGU, EMBASE, MEDLINE, PROMT, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

192 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
192 REFERENCES IN FILE CAPLUS (1907 TO DATE)
23 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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L41 192 L10

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L43 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:230222 CAPLUS Full-text
DOCUMENT NUMBER: 116:230222
TITLE: Photodynamic tetrapyrrole inducer defoliants and herbicides. Porphyrin-heme biosynthesis modulator insecticides.
INVENTOR(S): Rebeiz, Constantin A.
PATENT ASSIGNEE(S): University of Illinois, USA
SOURCE: PCT Int. Appl., 124 pp.
CODEN: PIXXD2
DOCUMENT TYPE: **Patent**
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

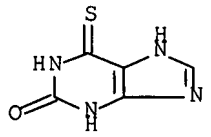
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9116820	A1	19911114	WO 1991-US3015	19910502
W: CA, JP, KR				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
US 5163990	A	19921117	US 1990-521119	19900503
US 5242892	A	19930907	US 1990-615413	19901119
EP 527186	A1	19930217	EP 1991-909022	19910502
R: BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL				
JP 06500989	T	19940127	JP 1991-508902	19910502

PRIORITY APPLN. INFO.:

US 1990-521119	A	19900503
US 1990-615413	A	19901119
US 1984-634932	B2	19840727
US 1985-754092	B1	19850715
US 1986-895529	A2	19860811
WO 1991-US3015	W	19910502

ED Entered STN: 13 Jun 1992
AB A composition, which induces accumulation of photodynamic tetrapyrroles in the foliage of plants, comprises a chlorophyll biosynthesis modulator , optionally in combination with δ-aminolevulinic acid. The composition is a herbicide, defoliant, or desiccant. An insecticidal composition which elevates endogenous tetrapyrrole levels in insects, comprises a porphyrin-heme biosynthesis modulator, optionally in combination with δ-aminolevulinic acid. Thus, application of a combination containing 20 mM δ-aminolevulinic acid and 15 mM 6-aminonicotinamide (modulator) defoliated tomato.
IT **2002-59-7**
RL: BIOL (Biological study)
(photodynamic chlorophyll biosynthesis modulator, as plant controlling

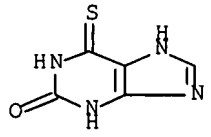
agent)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



L43 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:5495 CAPLUS Full-text
DOCUMENT NUMBER: 86:5495
TITLE: 2-Hydroxy-6-mercaptopurine
INVENTOR(S): Enoki, Kichiji; Genda, Yoshikazu; Hinoki, Yoshiaki
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: **Patent**
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51076294	A	19760701	JP 1975-3162	19741226
PRIORITY APPLN. INFO.:			JP 1975-3162 A	19741226

ED Entered STN: 12 May 1984
AB 2-Hydroxy-6-mercaptopurine (I) was prepared by heating 4(5)-thiocarbamoylimidazole-5(4)-carbamic acid esters in organic solvents. Thus, 5 g Me 4(5)-thiocarbamoylimidazole-5(4)-carbamate in DMF was stirred 2 hr at 140-50° to give 93% I.
IT **2002-59-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



L43 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:433086 CAPLUS Full-text
DOCUMENT NUMBER: 85:33086
TITLE: 2-Hydroxy-6-mercaptopurine
INVENTOR(S): Enoki, Kichiji; Tomita, Nobuo; Genda, Yoshikazu; Fukui, Takeo
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: **Patent**
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51008293	A	19760123	JP 1974-80779	19740716

PRIORITY APPLN. INFO.: JP 1974-80779 A 19740716
ED Entered STN: 12 May 1984
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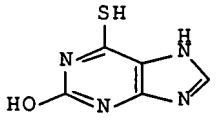
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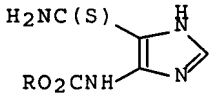
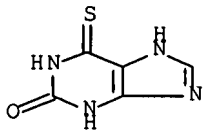

II

AB 2-Hydroxy-6-mercaptopurine (I) is prepared by cyclizing 4(5)-thiocarbamoylimidazole-5(4)-carbamate esters, e.g., II, with alkali or alcoholate in H2O or alcs. Thus, 2 g II (R = Me) was heated with 0.2 g NaOH in 20 ml H2O at 80-5° 3 hr to give 92.8% I. The yield was raised to 95.2% with 2 g NaOH or with 0.2 g Na in MeOH as the base.

IT **2002-59-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)

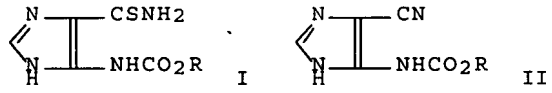


L43 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:433012 CAPLUS Full-text
DOCUMENT NUMBER: 85:33012
TITLE: 4(5)-Thiocarbamoylimidazole-5(4)-carbamate esters
INVENTOR(S): Enoki, Kichiji; Genda, Yoshikazu; Tomita, Nobuo; Fukui, Takeo
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: **Patent**
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

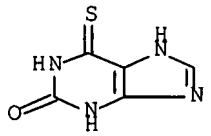
JP 51008271	A	19760123	JP 1974-80778	19740716

PRIORITY APPLN. INFO.: JP 1974-80778 A 19740716
ED Entered STN: 12 May 1984
GI



AB Title thioamides, e.g., I, are prepared by treating 4(5)-cyanoimidazole-5(4)-carbamate esters, e.g., II, with H2S in an organic solvent in the presence of aliphatic or alicyclic secondary amines. I are new compds. [substance claim] and are intermediates for 2-hydroxy-6-mercaptopurine (III). Thus, 8.3 g II (R = Me) and 0.1 g Et2NH in 50 ml DMF was treated with 3.3 g H2S at 50-5° 0.5 hr and heated 2 hr to give 90% I (R = Me). Iso-Bu2NH, piperidine, or pyrrolidine was also effective instead of Et2NH. Cyclization in 1% aqueous NaOH at 80-5° 3 hr gave 92.8% III.

IT **2002-59-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



L43 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1969:78011 CAPLUS Full-text
DOCUMENT NUMBER: 70:78011
TITLE: 6-Thioxanthine
INVENTOR(S): Yamazaki, Satohiro; Meguro, Takashi; Kumashiro, Izumi
PATENT ASSIGNEE(S): Ajinomoto Co., Inc.
SOURCE: Jpn. Tokkyo Koho, 2 pp.
CODEN: JAXXAD
DOCUMENT TYPE: **Patent**
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 43006224	B4	19680307	JP	19651125

ED Entered STN: 12 May 1984
AB 5-Amino-4-thiocarbamoylimidazole (I) is heated with urea. Thus, a mixture of 5 g. I and 10 g. urea is heated at 150-60° for 2 hrs., extracted with 0.5N NaOH, and the extract neutralized with AcOH to give 3.65 g. 6-thioxanthine. To prepare I, 50 g. 5-amino-4-carbamoylimidazole-HCl was mixed with 250 ml.

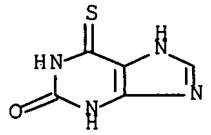
POCl3 at 85° for 4 hrs. The mixture was cooled to give 19.6 g. 5-amino-4-cyanoimidazole (II), m. 128-9° (decomposition). A solution of 20 g. II in 360 ml. MeOH was mixed with 50 ml. KOH-MeOH solution (containing 155 g. KOH). The solution was saturated with H2S at room temperature, heated in a sealed tube at 100° for 2 hrs., and acidified with HOAc to give I.HOAc, which was dissolved in 2N HCl and the solution concentrated to give 15 g. I.HCl.

IT **2002-59-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



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DICTIONARY FILE UPDATES:  11 MAR 2007  HIGHEST RN 926007-42-3

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L11  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2007 ACS on STN
RN   2487-40-3  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Xanthine, 2-thio- (6CI, 7CI, 8CI)
OTHER NAMES:
CN   2,3-Dihydro-2-thioxo-9H-purin-6(1H)-one
CN   2-Mercapto-6-hydroxypurine
CN   2-Mercaptohypoxanthine
CN   2-Thio-6-hydroxypurine
CN   2-Thioxanthine
CN   6-Hydroxy-2-mercaptopurine
CN   6-Hydroxypurine-2-thiol
CN   NSC 36822
CN   NSC 680828
DR   69-90-9, 3240-64-0, 5167-21-5, 6050-40-4
MF   C5 H4 N4 O S
CI   COM
LC   STN Files:   AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT,
       CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, EMBASE, GMELIN*, IFICDB,
       IFIPAT, IFIUDB, IPA, MEDLINE, PROMT, RTECS*, TOXCENTER, USPAT2,
       USPATFULL
         (*File contains numerically searchable property data)
     Other Sources:   EINECS**, NDSL**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
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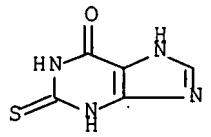


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

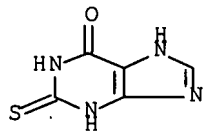
154 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
154 REFERENCES IN FILE CAPLUS (1907 TO DATE)
20 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> => d ibib ed abs hitstr 48-52

L46 ANSWER 48 OF 52 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1969:524508 CAPLUS Full-text
DOCUMENT NUMBER: 71:124508
TITLE: 2-Mercaptohypoxanthine
INVENTOR(S): Kawashima, Hideaki; Kumashiro, Izumi
PATENT ASSIGNEE(S): Ajinomoto Co., Inc.
SOURCE: Jpn. Tokkyo Koho, 2 pp.
CODEN: JAXXAD
DOCUMENT TYPE: **Patent**
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 44010790	B4	19690519	JP	19660211

ED Entered STN: 12 May 1984
AB Manufacture of the title product (I) by heating 6-alkoxypurine 3-oxide (II) with an excess of thioacetic acid (III) is described. Thus, 1 g. II (alkyl = Me) in 20 ml. III is heated 4 hrs. at 98° to give 89% I, m. >360°.
IT **2487-40-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)

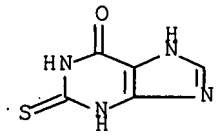


L46 ANSWER 49 OF 52 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1968:410477 CAPLUS Full-text
DOCUMENT NUMBER: 69:10477
TITLE: Purine derivatives

INVENTOR(S): Fujimoto, Yasuo; Teranishi, Masayuki
PATENT ASSIGNEE(S): Kyowa Fermentation Industry Co., Ltd.
SOURCE: Jpn. Tokkyo Koho, 7 pp.
CODEN: JAXXAD
DOCUMENT TYPE: **Patent**
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 42020067	B4	19671006	JP	19640118

ED Entered STN: 12 May 1984
AB 2-(Phenylazocyano)acetamide (5.7 g.) and 7 g. formamidine acetate is refluxed 3 hrs. in 50 ml. Et Cellosolve, then a mixture of 20 ml. formamide and 2 to 4 g. Na hydrosulfite are added at 110-30° during 20 min., the mixture is kept at 110-30° for 30 min., then heated at 170-90° for 3 hrs., 200-300 ml. H2O added and filtered when hot, and the filtrate is treated with C, concentrated, and kept in a refrigerator overnight to give 2.4 g. hypoxanthine. Similarly prepared are 2-mercaptohypoxanthine, guanine, xanthine, 2-phenyl-6-hydroxypurine, 2-benzylhypoxanthine, 2-β-pyridyl-6-hydroxypurine, and 2-methyl-6-hydroxypurine.
IT **2487-40-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L46 ANSWER 50 OF 52 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:465567 CAPLUS Full-text
DOCUMENT NUMBER: 65:65567
ORIGINAL REFERENCE NO.: 65:12218f-g
TITLE: Preparation of purine and derivatives
PATENT ASSIGNEE(S): Kyowa Fermentation Industry Co., Ltd.
SOURCE: 7 pp.
DOCUMENT TYPE: **Patent**
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1425603		19660121	FR	
PRIORITY APPLN. INFO.:			JP	19640118

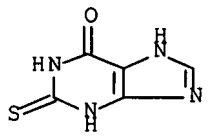
ED Entered STN: 22 Apr 2001
AB Derivs. of purine were prepared by treating an α-arylazocyanoacetamide (I) with urea, thiourea, or an amidine. The condensation was followed by a catalytic or chemical reduction and a heating in the presence of a cyclizing agent such as formamide. Thus, a mixture of 5.7 parts 2-

phenylazocyanoacetamide, 7 parts formamidine acetate, and 50 parts Et Cellosolve was boiled 3 hrs. then 20 parts formamide and 2.4 parts Na hydrosulfite added, and the mixture stirred 20 min. at 110-30° and 3 hrs. at 170-90°. Cooling, treating with 200-300 parts H2O, and filtering with C gave 2.4 parts free hypoxanthine. Similarly were prepared 2-mercaptohypoxanthine from ethyl 2-(p-hydroxyphenylazo)cyanoacetate and thiourea, guanine from ethyl 2-(pmethylphenylazo)cyanoacetate and guanidine carbonate, xanthine from ethyl 2-(m-phenylnitroazo)cyanoacetate and urea, 2-(methylthio)hypoxanthine from N-(2- phenylazocyanoacetyl)hydroxylamine and S-methylthiourea sulfate, and 2-methylhypoxanthine from 2-phenylazocyanoacetamide and acetamide-HCl.

IT **2487-40-3P**, Xanthine, 2-thio-
RL: PREP (Preparation)
(manufacture of)

RN 2487-40-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L46 ANSWER 51 OF 52 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:27626 CAPLUS Full-text

DOCUMENT NUMBER: 64:27626

ORIGINAL REFERENCE NO.: 64:5116b-c

TITLE: Hypoxanthine

PATENT ASSIGNEE(S): Kyowa Fermentation Industry Co., Ltd.

SOURCE: 15 pp.

DOCUMENT TYPE: **Patent**

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1415149		19651022	FR 1964-995256	19641117
PRIORITY APPLN. INFO.:			JP	19631118

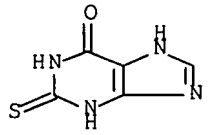
ED Entered STN: 22 Apr 2001

AB The title compound (I) was prepared by nitrosation of 4-amino-6-hydroxypyrimidine (II), reduction of the 5-nitroso compound, and ring closure in presence of HCONMe2 (III) in one stage. Thus, II 11.1 was added to a mixture of NaNO2 7.3 and III 120, cooled to 0-4°, 98% HCO2H 7 added gradually, maintained at 10° for nitrosation, heated to 120-50°, Na2S2O4 added gradually within 10 min., refluxed at 180° for 1 hr., cooled, H2O added, and the precipitate filtered off to give 9.2 parts I.

IT **2487-40-3P**, Xanthine, 2-thio-
RL: PREP (Preparation)
(preparation of)

RN 2487-40-3 CAPLUS

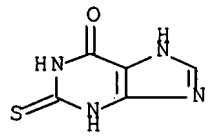
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L46 ANSWER 52 OF 52 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:27625 CAPLUS Full-text
DOCUMENT NUMBER: 64:27625
ORIGINAL REFERENCE NO.: 64:5115h,5116a-b
TITLE: Purine derivatives
PATENT ASSIGNEE(S): Kyowa Fermentation Industry Co., Ltd.
SOURCE: 12 pp.
DOCUMENT TYPE: **Patent**
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1415224		19651022	FR 1964-996273	19641125
PRIORITY APPLN. INFO.:			JP	19631126

ED Entered STN: 22 Apr 2001
AB An improved process is reported for the reduction of o-aminoazopyrimidines and cyclization of the diamines produced to the aminopyrimidines. A cathode mixture containing 5.3 parts 4-amino-5-phenylazo-6-hydroxypyrimidine suspended in 150 vols. 50% HCO2H was electrolyzed for 2.5 hrs. using a Pb cathode (of area 27 cm.2 per each 150 vols. of liquid) and a C anode, at a c.d. of 50-60 amp./dm.2 at 90-105° until the initial color had disappeared. The resulting solution was refluxed for 8 hrs. to give 2.5 parts hypoxanthine (I). A similar reduction and cyclization was carried out in 3:1 90% HCO2H-HCONH2. Reduction and cyclization of 5.4 parts 4,6-diamino-5- phenylazopyrimidine similarly gave 2.7 parts adenine while 2,4-diamino-6-hydroxy-5-phenylazopyrimidine gave guanine. Other compds. prepared from the corresponding phenylazopyrimidines were (compound and % yield given): isoguanine, 81; 2,6-diaminopurine, 80; 2-aminopurine, 73; 2-diethylaminopurine, 75; 2-methylhypoxanthine, 75; 2-hydroxy-6- methylpurine, 71; 2-amino-6-methylpurine, 74; 2-mercaptoxanthine, 75; 2-mercapto-, 80, and 2-methylthioadenine, 79; 2-methylguanine 81; 1,3-diethylxanthine, 72.
IT **2487-40-3P**, Xanthine, 2-thio-
RL: PREP (Preparation)
(preparation of)
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



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DICTIONARY FILE UPDATES:  11 MAR 2007  HIGHEST RN 926007-42-3

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L12  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2007 ACS on STN
RN   5437-25-2  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   1H-Purine-2,6-dithione, 3,9-dihydro-  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   1H-Purine-2,6-dithione, 3,7-dihydro- (9CI)
CN   Xanthine, dithio- (6CI, 7CI, 8CI)
OTHER NAMES:
CN   2,6-Dimercaptopurine
CN   2,6-Dithiopurine
CN   2,6-Dithioxanthine
CN   2,6-Dithioxo-1,2,3,6-tetrahydro-9H-purine
CN   Dithioxanthine
CN   NSC 15989
CN   NSC 685799
CN   Purine-2,6-dithiol
DR   7390-61-6
MF   C5 H4 N4 S2
CI   COM
LC   STN Files:   BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
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         (**Enter CHEMLIST File for up-to-date regulatory information)
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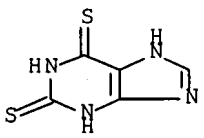


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

90 REFERENCES IN FILE CA (1907 TO DATE)
90 REFERENCES IN FILE CAPLUS (1907 TO DATE)
12 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

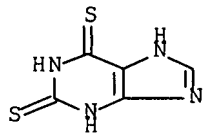
=> => d ibib ed abs hitstr 12-16

L48 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:97840 CAPLUS Full-text
DOCUMENT NUMBER: 84:97840
TITLE: Photothermographic recording material
INVENTOR(S): White, Richard Lawson
PATENT ASSIGNEE(S): Eastman Kodak Co., USA
SOURCE: Ger. Offen., 32 pp.
CODEN: GWXXBX
DOCUMENT TYPE: **Patent**
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 2519585	A1	19751106	DE 1975-2519585		19750502
CA 1043617	A1	19781205	CA 1975-223845		19750429
BE 828685	A1	19751103	BE 1975-156028		19750502
FR 2269736	A1	19751128	FR 1975-13777		19750502
JP 50151138	A	19751204	JP 1975-52590		19750502
GB 1501005	A	19780215	GB 1975-18493		19750502
PRIORITY APPLN. INFO.:			US 1974-466331	A	19740502

ED Entered STN: 12 May 1984
AB Photothermog. recording materials giving images with a black tone and a high contrast are composed of a support having coated thereon a heat-developable, light-sensitive composition containing a Ag halide, a Ag salt of a heterocyclic thione, such as 3-carboxymethyl-4-methyl-4-thiazoline-2- thione Ag salt (I), an organic reducing agent, such as tert- butylhydroquinone, a heterocyclic mercapto compound as a toner, and a binder. Thus, an aqueous dispersion of I containing 9.6 mg Ag/ml 7, a 10% MeOH solution of tert-butylhydroquinone 1, a gelatin-AgI emulsion (21.2 mg Ag/ml and 0.06 μ average grain size) 0.4, nonylphenoxyglycidol 0.4 ml, and 3-mercapto-1,2,4-triazole 1 mg were mixed, coated on a support, dried, imagewise exposed to unfiltered tungsten light, and developed from 2-8 sec at 160° to give an image d. ≥1. The blue reflection d. and the visible reflection d. were then determined and their difference determined to be 0.12, which indicated that 3-mercapto-1,2,4-triazole was an especially good toner.
IT **5437-25-2**
RL: USES (Uses)
(photothermog. copying compns. containing, for improved tone and contrast)
RN 5437-25-2 CAPLUS

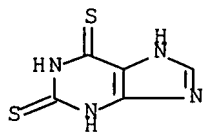
CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



L48 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:18763 CAPLUS Full-text
DOCUMENT NUMBER: 82:18763
TITLE: Process and bath for increasing the polymer deposition velocity in electrolytic coating
INVENTOR(S): Dudley, Michael A.
PATENT ASSIGNEE(S): Canada Wire and Cable Co. Ltd.
SOURCE: Ger. Offen., 22 pp.
CODEN: GWXXBX
DOCUMENT TYPE: **Patent**
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2364936	A1	19740711	DE 1973-2364936	19731228
CA 976290	A1	19751014	CA 1972-160228	19721229
GB 1425389	A	19760218	GB 1973-58923	19731219
US 4020028	A	19770426	US 1974-429771	19740102
US 4136074	A	19790123	US 1975-630944	19751112
PRIORITY APPLN. INFO.:			CA 1972-160228 A	19721229
			US 1974-429771 A3	19740102

ED Entered STN: 12 May 1984
AB The rate of polymer deposition on a metal anode during electrophoretic coating with an epoxy ester, acrylic, or alkyd resin was increased by adding 0.01-2.0% Ac2CH2 [123-54-6], 1H-1,2,4-triazole-3-thiol [3179-31-5], 3-mercapto-1,2-propanediol [96-27-5], 2-mercaptobenzoselenazole [10486-58-5], phenol [108-95-2], di(2-pyridyl)amine [1202-34-2], 2-mercaptopyrimidine [1450-85-7], or a similar compound to the baths. Thus, the rate of deposition of an epoxy ester resin on an Al anode was increased 70.6% by adding 0.2% Ac2CH2 to the bath.
IT **5437-25-2**
RL: USES (Uses)
(electrophoresis baths containing, for rapid coating)
RN 5437-25-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



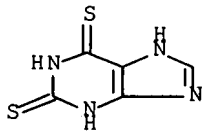
L48 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:493614 CAPLUS Full-text
DOCUMENT NUMBER: 73:93614
TITLE: Use of silver pi-complex stabilizers
INVENTOR(S): Dunham, Kenneth R.
SOURCE: Def. Publ. U. S. Pat. Off. T, 22 pp. From: Off. Gaz. 1970, 877(3), 491.
CODEN: USXXBN
DOCUMENT TYPE: **Patent**
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 877011		19700818	US	19700211

ED Entered STN: 12 May 1984

AB A developed image in a photographic element containing a photographic π-complex of a Ag salt, especially a water-soluble salt and an organic compound, such as a Ag cycloheptatriene π-complex, can be stabilized with a Ag π-complex stabilizer, such as a thiadiazole, purine, benzimidazole, imidazoline, or pyrimidine. Such stabilizers are desirably odorless and form a stable Ag mercaptide. The photographic element can contain light-sensitive TiO2. An image in an exposed photographic element containing a photographic Ag π-complex, a Ag halide developing agent, and a Ag π-complex stabilizer can be developed and stabilized by heating the photographic element.

IT **5437-25-2**
RL: USES (Uses)
(photographic processing solns. containing, for silver complex print-out emulsions)
RN 5437-25-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



L48 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:105870 CAPLUS Full-text
DOCUMENT NUMBER: 72:105870
TITLE: Development and stabilization of photographic films
INVENTOR(S): Cole, Roger M.
PATENT ASSIGNEE(S): Eastman Kodak Co.
SOURCE: Ger. Offen., 28 pp.
CODEN: GWXXBX
DOCUMENT TYPE: **Patent**
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1923824	A	19691211	DE 1969-1923824	19690509

US 3615511	A	19711026	US 1968-731275	19680522
FR 2009092	A5	19700130	FR 1969-16527	19690521
GB 1275074	A	19720524	GB 1969-1275074	19690522

PRIORITY APPLN. INFO.: US 1968-731275 A 19680522

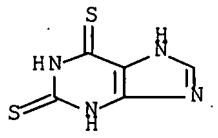
ED Entered STN: 12 May 1984

AB Fog formation during development or stabilization of imagewise exposed and optionally photodeveloped Ag halide recording materials of the internal image type can be avoided by use of developer solns. which are substantially free of strong Ag halide solvents and which contain, in addition to the usual developer compds. 1 + 10-5-2 + 10-3 mole (1 + 10-5-4 + 10-3 mole for use in conjunction with a process involving a Ag halide bleach solution) of a Ag complex forming compound which contains ≥1 group capable of undergoing covalent bond formation with Ag (e.g., a mercapto or imino group) and 1 group containing a π bond (e.g. the :I:C: bond). Stable images or copies are obtained with this type of developer solution (followed by fixation and washing) after exposure of print-out recording materials or after photodevelopment of direct copying photographic recording materials. Thus, several strips of a direct copying Ag halide emulsion were exposed (10-4 sec, Xe lamp) through a step wedge and subsequently photodeveloped. The strips were developed (60 sec) in developer (A) containing H2O 800 ml, N-methyl-p-aminophenol sulfate 6, Na isoascorbate 40, KBr 1, K metabo rate 40, 4-methyl-1-phenyl-3-pyrazolidinone 1, 1-phenyl-5-mercaptoterazole (I) 0.1 g, and H2O to 1 l., immersed (10 sec) in an AcOH stop bath, fixed (2 min) in a Na2S2O3 solution, and washed (5 min) in running H2O and showed a background d. and image d. of 0.67 and 1.01, resp., vs. 0.48 and 0.46 for the control developed in I-free developer A. The presence of I in the developer solution prevented image reversal and enhanced the development of the highly exposed image areas. The resulting neg. image corresponded to that which would have been obtained by the customary photodevelopment used for direct copying recording materials.

IT **5437-25-2**
RL: USES (Uses)
(photographic developing solns. containing, for prevention of fog formation)

RN 5437-25-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



L48 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	1969:524506 CAPLUS Full-text
DOCUMENT NUMBER:	71:124506
TITLE:	2,6- and 6,8-Dimercaptopurines
INVENTOR(S):	Kawashima, Hideaki; Kumashiro, Izumi
PATENT ASSIGNEE(S):	Ajinomoto Co., Inc.
SOURCE:	Jpn. Tokkyo Koho, 2 pp. CODEN: JAXXAD
DOCUMENT TYPE:	**Patent**
LANGUAGE:	Japanese
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 44010789	B4	19690516	JP	19660210

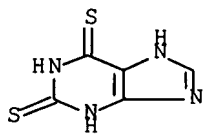
ED Entered STN: 12 May 1984

AB Heating 6-chloropurine 3-oxide (I) with an excess of thioacetic acid (II) is described. Thus, 1 g. I is heated 6 hrs. at 98° with 25 g. II, the resulting yellow powder dissolved in dilute NH4OH and passed through a column of 300 ml. Dowex 50W-X4, and the column eluted with H2O and then with N NH4OH to give 14% 6,8-dimercaptopurine and 51% 2,6- dimercaptopurine, successively.

IT **5437-25-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 5437-25-2 CAPLUS

CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



REFERENCES FOR ALL THE OTHER HITS

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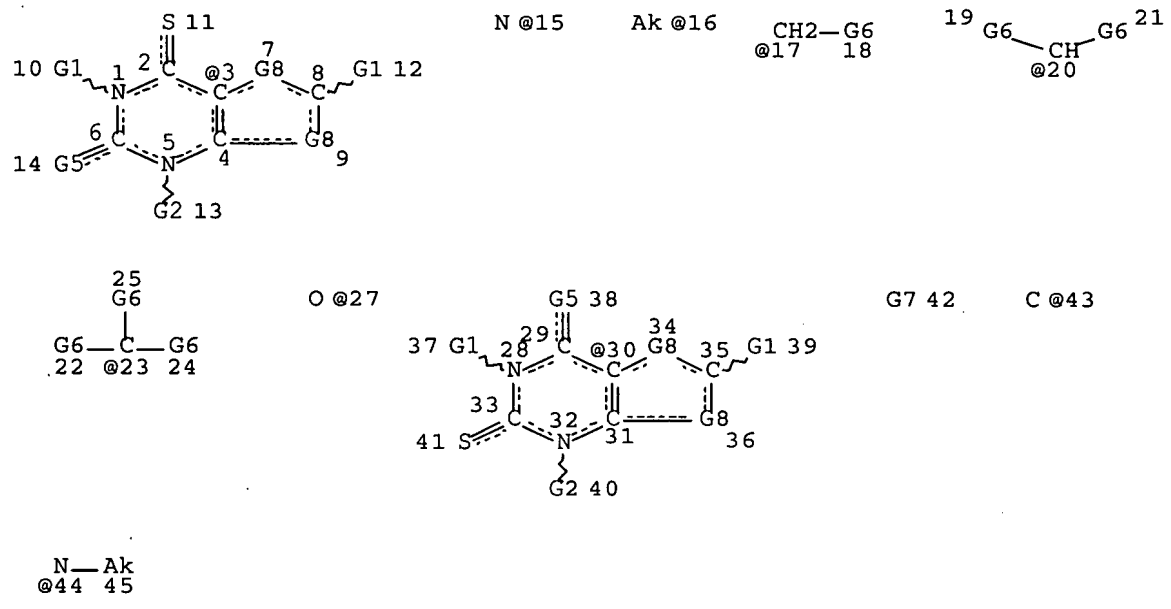
L4 STR



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VAR G8=15/NH/44

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FILE LAST UPDATED: 11 Mar 2007  (20070311/ED)

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L57 116 L16 NOT L17

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L57 ANSWER 1 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:706960 CAPLUS Full-text
DOCUMENT NUMBER: 139:230796
TITLE: Synthesis of new purine derivatives
INVENTOR(S): Miyamoto, Kenichi; Sawanishi, Hiroyuki; Suzuki, Koichi; Yamamoto, Manabu; Shimura, Susumu
PATENT ASSIGNEE(S): Lotte Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
JP 2003252875	A	20030910	JP 2002-58098		20020304	<--
KR 2003072251	A	20030913	KR 2003-13401		20030304	<--
PRIORITY APPLN. INFO.:			JP 2002-58098	A	20020304	<--

OTHER SOURCE(S): MARPAT 139:230796
ED Entered STN: 10 Sep 2003
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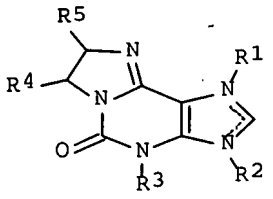

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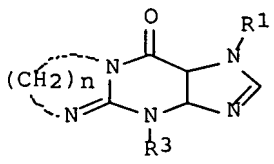
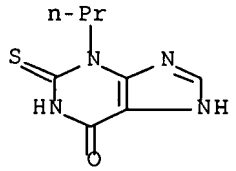


II

AB The patent relates to the preparation of purine derivs. and salts for pharmaceutical uses such as PDE IV isoenzyme inhibitor. The purine derivs. have the following formula (I) wherein R1, R2, R3 are hydrogen, or hydroxy, low alkyloxy, acyl substituted C1-C6 alkyl, or phenyl; and R4, and R5 are independently hydroxy, low alkyloxy, acyl substituted C1-C6 alkyl, or Ph group; and pharmaceutically compatible salts. The purine derivs. and pharmaceutically compatible salts may have the following formula (II) wherein R1, R2 are hydrogen, or hydroxy, low alkyloxy, acyl substituted C1-C6 alkyl, or phenyl; and n = 2 or 3. Thus, 8-methyl-4-propyl-4,5,7,8-tetrahydro-1H-imidazole-[2,1,i]purine-5-one prepared from 6-[(2-hydroxy-1-methyl)ethyl]amino-3-propylpurine-2-one in presence of triethylamine, and methanesulfonyl chloride was evaluated for PDE I test and gave greater activity than the control using Denoufylline.

IT **156733-29-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in preparation of new purine derivs.)
RN 156733-29-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-propyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 2 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:723414 CAPLUS Full-text
DOCUMENT NUMBER: 138:137075
TITLE: Synthesis and cyclic AMP phosphodiesterase 4 isoenzyme inhibitory activity of heterocycle condensed purines
AUTHOR(S): Suzuki, Hirokazu; Yamamoto, Manabu; Shimura, Susumu; Miyamoto, Ken-ichi; Yamamoto, Kenji; Sawanishi, Hiroyuki
CORPORATE SOURCE: Department of Synthetic Chemistry, Hokuriku University, Kanazawa, 920-1181, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(9), 1163-1168
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:137075
ED Entered STN: 24 Sep 2002
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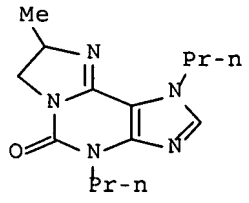


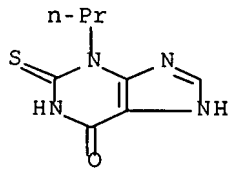
I

AB To reverse the adverse reactions of alkylxanthines and to develop novel inhibitors of cAMP phosphodiesterase 4 (PDE4), a series of heterocycle [a]-, [b]-, [c,d]-, and [i]-condensed purines were designed and synthesized. Although all compds. did not display PDE1 and PDE3 inhibitory activities, several heterocycle [i]-condensed purines strongly inhibited PDE4. Especially, dl-3,4-dipropyl-8-methyl-4,5,7,8-tetrahydro-1H- imidazo[2,1-i]purin-5-one (I) exhibited comparable PDE4 inhibitory activity (IC50=1.9 μM) to rolipram and denbufylline (DBF).
IT **156733-29-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heterocycle condensed purines from purine and pyrimidine derivs. and their activity as cAMP phosphodiesterase 4 isoenzyme inhibitors)

RN 156733-29-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-propyl-2-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 3 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:502824 CAPLUS Full-text

DOCUMENT NUMBER: 137:63122

TITLE: Preparation of purine derivatives or therapeutic use as phosphodiesterase IV inhibitors

INVENTOR(S): Chasin, Mark; Cavalla, David J.; Hofer, Peter; Gehrig, Andre; Wintergerst, Peter

PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg

SOURCE: U.S., 34 pp., Cont.-in-part of U.S. Ser. No. 285,473. CODEN: USXXAM

DOCUMENT TYPE: Patent

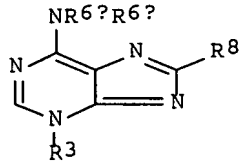
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 21

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6413975	B1	20020702	US 2000-539571	20000331 <--
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
HU 200200938	A2	20021028	HU 2002-938	20000331 <--
JP 2001316314	A	20011113	JP 2000-136383	20000509 <--
US 2003073834	A1	20030417	US 2002-62280	20020201 <--
PRIORITY APPLN. INFO.:			US 1999-285473	A2 19990402 <--
			IN 1994-CA514	A1 19940630 <--
			US 1997-963054	A2 19971103 <--
			US 1997-875487	A2 19971113 <--
			US 1998-151949	A2 19980911 <--
			US 1998-210556	A2 19981211 <--
			US 1998-210557	A2 19981211 <--
			US 1999-227057	A2 19990107 <--
			US 1999-237638	A2 19990126 <--
			US 1999-361196	A2 19990726 <--
			US 2000-506624	A2 20000218 <--
			US 2000-539571	A2 20000331 <--
			US 2000-547575	A2 20000412 <--
			US 2000-547898	A2 20000412 <--
			US 2000-636146	A2 20000810 <--
			US 2000-724321	B1 20001128 <--

OTHER SOURCE(S): MARPAT 137:63122
ED Entered STN: 04 Jul 2002
GI



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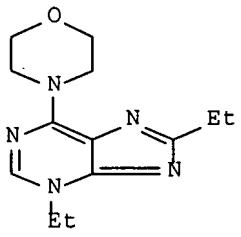
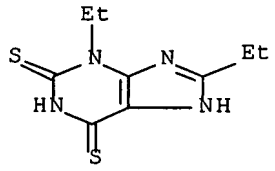


II

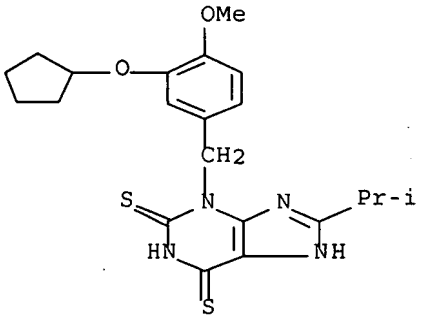
AB Purines, such as I [R3, R6a, R6b, R8 = H, alkyl, alkenyl, cycloalkyl, aryl, arylalkyl, etc.], were prepared for pharmaceutical use as phosphodiesterase IV (PDE IV) inhibitors. Thus, 3,8-diethyl-6-morpholino- 3H-purine (II) was prepared by conversion of 3,8-diethyl-2-thioxanthine to 3,8-diethylhypoxanthine using 2N NaOH and nickel aluminum alloy, reaction of 3,8-diethylhypoxanthine to 3,8-diethyl-6-thiohypoxanthine using phosphorus pentasulfide in pyridine and, finally, reaction of 3,8-diethyl-6-thiohypoxanthine with morpholine. The prepared purine derivs. were assayed for PDE IV inhibition.

IT **162278-92-4P**, 3,8-Diethyl-2,6-dithioxanthine **162279-04-1P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of purine derivs. for therapeutic use as phosphodiesterase IV inhibitors)

RN 162278-92-4 CAPLUS
CN 1H-Purine-2,6-dithione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)

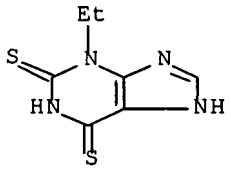


RN 162279-04-1 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)

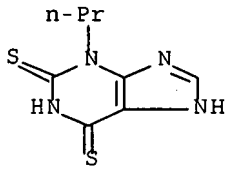


IT **162278-87-7P 162278-88-8P 162278-89-9P**
162278-90-2P 162278-91-3P 162278-93-5P
162278-94-6P 162279-01-8P 162279-02-9P
162279-05-2P 162279-06-3P 162279-07-4P
162279-08-5P 162279-09-6P 162279-10-9P
300783-48-6P 300783-53-3P 439694-45-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of purine derivs. for therapeutic use as phosphodiesterase IV inhibitors)

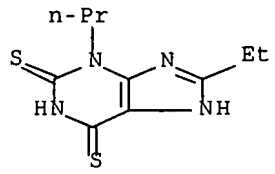
RN 162278-87-7 CAPLUS
CN 1H-Purine-2,6-dithione, 3-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



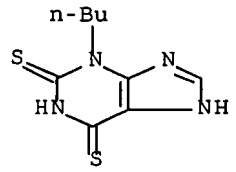
RN 162278-88-8 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-propyl- (9CI) (CA INDEX NAME)



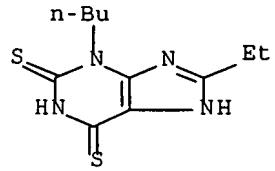
RN 162278-89-9 CAPLUS
CN 1H-Purine-2,6-dithione, 8-ethyl-3,7-dihydro-3-propyl- (9CI) (CA INDEX NAME)



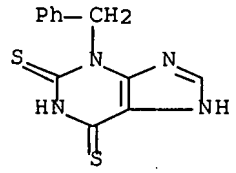
RN 162278-90-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3-butyl-3,7-dihydro- (9CI) (CA INDEX NAME)



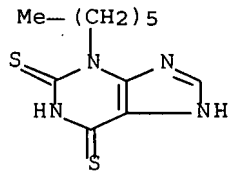
RN 162278-91-3 CAPLUS
CN 1H-Purine-2,6-dithione, 3-butyl-8-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



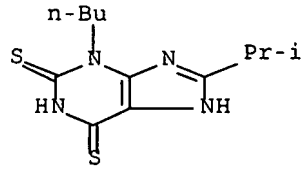
RN 162278-93-5 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



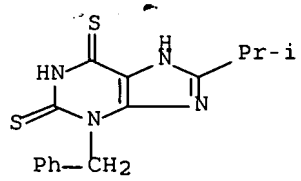
RN 162278-94-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3-hexyl-3,7-dihydro- (9CI) (CA INDEX NAME)



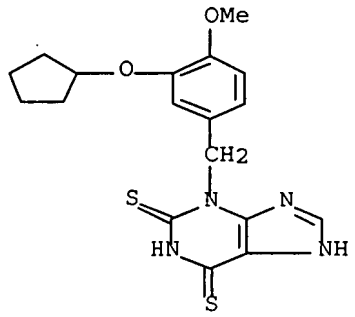
RN 162279-01-8 CAPLUS
CN 1H-Purine-2,6-dithione, 3-butyl-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



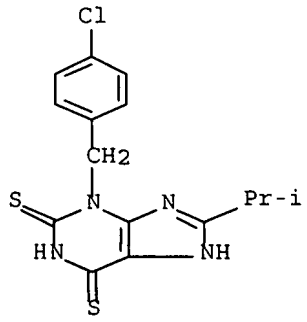
RN 162279-02-9 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



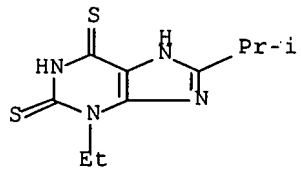
RN 162279-05-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro- (9CI) (CA INDEX NAME)



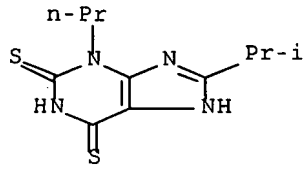
RN 162279-06-3 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[(4-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



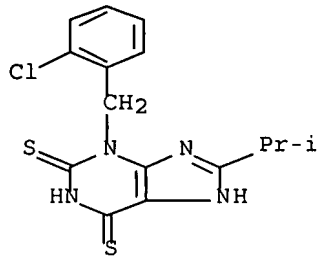
RN 162279-07-4 CAPLUS
CN 1H-Purine-2,6-dithione, 3-ethyl-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



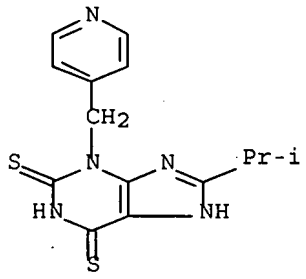
RN 162279-08-5 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-propyl- (9CI) (CA INDEX NAME)



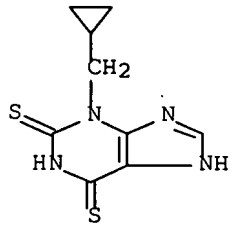
RN 162279-09-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[(2-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



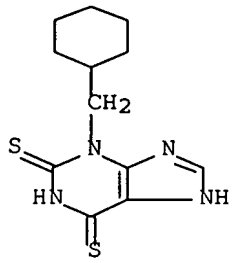
RN 162279-10-9 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



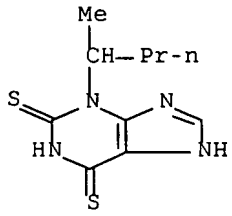
RN 300783-48-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3-(cyclopropylmethyl)-3,7-dihydro- (9CI) (CA INDEX NAME)



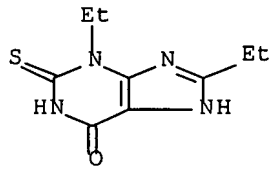
RN 300783-53-3 CAPLUS
CN 1H-Purine-2,6-dithione, 3-(cyclohexylmethyl)-3,7-dihydro- (9CI) (CA INDEX NAME)



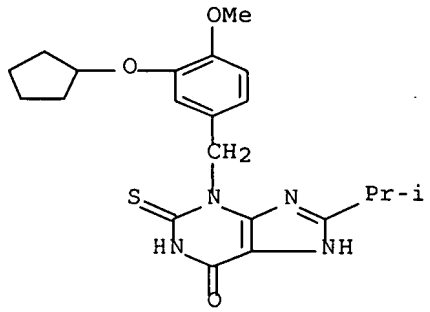
RN 439694-45-8 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-(1-methylbutyl)- (9CI) (CA INDEX NAME)



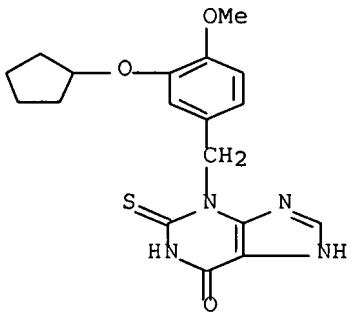
IT **162278-04-8**, 3,8-Diethyl-2-thioxanthine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of purine derivs. for therapeutic use as phosphodiesterase IV inhibitors)
RN 162278-04-8 CAPLUS
CN 6H-Purin-6-one, 3,8-diethyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



IT **300781-30-0P**, 3-(3-Cyclopentyloxy-4-methoxybenzyl)-8-isopropyl-2-thioxanthine **300781-35-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of purine derivs. for therapeutic use as phosphodiesterase IV inhibitors)
RN 300781-30-0 CAPLUS
CN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,2,3,7-tetrahydro-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)

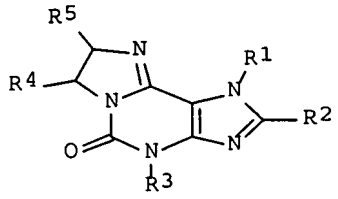


RN 300781-35-5 CAPLUS
CN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 86 THERE ARE 86 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 4 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:485205 CAPLUS Full-text
DOCUMENT NUMBER: 137:201279
TITLE: Imidazo[2,1-i]purin-5-ones and Related Tricyclic Water-Soluble Purine Derivatives: Potent A2A- and A3-Adenosine Receptor Antagonists
AUTHOR(S): Mueller, Christa E.; Thorand, Mark; Qurishi, Ramatullah; Diekmann, Martina; Jacobson, Kenneth A.; Padgett, William L.; Daly, John W.
CORPORATE SOURCE: Pharmaceutical Institute Poppelsdorf, University of Bonn, Bonn, Germany
SOURCE: Journal of Medicinal Chemistry (2002), 45(16), 3440-3450
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:201279
ED Entered STN: 28 Jun 2002
GI



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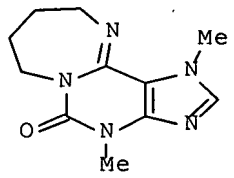


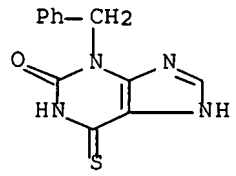
II

AB A series of tricyclic imidazo[2,1-i]purinones I [R1, R4 = H, Me; R2 = H, Ph, (E)-PhCH:CH; R3 = H, Me, PhCH2; R5 = H, Me, Et] and ring-enlarged analogs, e.g. II, derived from xanthine derivs. were prepared as adenosine receptor (AR) antagonists. In comparison with xanthines, these tricyclic compds. exhibited increased water solubility due to a basic nitrogen atom, which can be protonated under physiol. conditions. A new capillary electrophoresis method was developed for the determination of the enantiomeric purity of selected chiral products using native and modified β-cyclodextrins as chiral discriminators. The compds. were investigated in radioligand binding assays at rat brain A1 and A2A ARs. Selected I were addnl. investigated in

radioligand binding assays at human recombinant A3 ARs and in functional studies (adenylate cyclase assays) at A1 ARs of rat fat cell membranes, A2A ARs of rat PC 12 cell membranes, and mouse A2B ARs of NIH 3T3 cell membranes, and showed the structure-activity relationships similar to those of the corresponding xanthine derivs. The 2-styrylimidazopurinones I [R1 = H, Me; R2 = (E)-PhCH:CH; R3 = Me; R4 = H, R5 = Et] were less potent at A2A ARs as compared to 8-styrylxanthine derivs. The most potent compound at A2A ARs was (S)-I [R1 = R3 = Me, R2 = (E)-PhCH:CH, R4 = H, R5 = Et; (III)] exhibiting a Ki value of 424 nM at rat A2A ARs. III was also highly selective for A2A receptors vs A1 and A3 ARs; however, the selectivity vs A2B ARs was low. Among the 1-unsubstituted (2-phenyl)imidazopurinones, the most potent A3 antagonist was (R)-I (R1 = R4 = H, R2 = Ph, R3 = Me, R5 = Et) exhibiting a Ki value of 2.3 nM and high selectivity for A3 receptors vs all other AR subtypes.

IT **19844-94-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of imidazopurinones and ring-enlarged analogs as adenosine receptor antagonists via thiation of xanthines, methylation of thioxopurinones, coupling of (methylthio)purinones with amino alcs., and heterocyclization)

RN 19844-94-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(phenylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 5 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:90055 CAPLUS Full-text
DOCUMENT NUMBER: 136:131252
TITLE: Cationic materials and methods for covalent bonding nucleic acids to high purity silica surfaces
INVENTOR(S): Lyles, Mark B.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 9 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008237	A2	20020131	WO 2001-US23079	20010720 <--
WO 2002008237	A3	20021107		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,
VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
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BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2001076023	A5	20020205	AU 2001-76023		20010720 <--
US 2002103350	A1	20020801	US 2001-910697		20010720 <--
US 6855817	B2	20050215			
EP 1305328	A2	20030502	EP 2001-953590		20010720 <--
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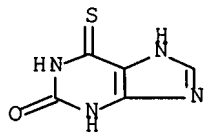
US 2005148067	A1	20050707	US 2005-57440		20050214 <--
PRIORITY APPLN. INFO.:			US 2000-220096P	P	20000721 <--
			US 2001-910697	A	20010720 <--
			WO 2001-US23079	W	20010720 <--

ED Entered STN: 01 Feb 2002

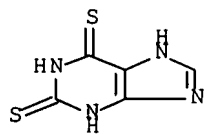
AB Surfaces containing high purity silica (silicon dioxide) exhibit high loading potential for nucleic acids. Formulations containing nucleic acids and materials which mask the electrostatic interactions between the nucleic acids and surfaces are disclosed. By masking the phosphate charges of the nucleic acids, undesired interactions may be minimized or eliminated, thereby allowing the covalent bonding of the nucleic acids to the surface to proceed. The use of such formulations addnl. minimizes nonspecific binding of the nucleic acids to the surface. Examples of materials to be included in such formulations include cations, xanthines, hexoses, purines, arginine, lysine, polyarginine, polylysine, and quaternary ammonium salts.

IT **2002-59-7**, 6-Thioxanthine **5437-25-2**, 2,6-Dithiopurine
91725-06-3
RL: NUU (Other use, unclassified); USES (Uses)
(cationic materials and methods for covalent bonding nucleic acids to high purity silica surfaces)

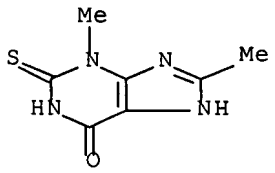
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



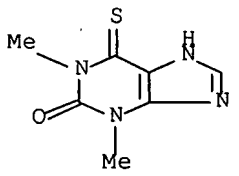
RN 5437-25-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



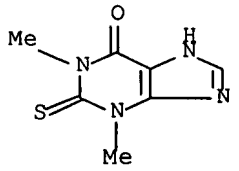
RN 91725-06-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3,8-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



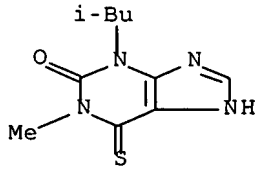
L57 ANSWER 6 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:413184 CAPLUS Full-text
DOCUMENT NUMBER: 135:251414
TITLE: Structural predictions of adenosine 2B antagonist affinity using molecular field analysis
AUTHOR(S): Song, Yuqing; Coupar, Ian M.; Iskander, Magdy N.
CORPORATE SOURCE: Department of Medicinal Chemistry, Victorian College of Pharmacy, Monash University, Parkville, 3052, Australia
SOURCE: Quantitative Structure-Activity Relationships (2001), 20(1), 23-30
CODEN: QSARDI; ISSN: 0931-8771
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 08 Jun 2001
AB 3D structural evaluation of the adenosine 2B (A2B) antagonist binding site is the major aim for developing specific selective antagonists. In an attempt to deduce structural properties of the antagonist site, a pharmacophore model was developed using 85 known A2B antagonists. The mol. mechanics optimization methods were used to deduce the likely binding conformations of the antagonists at the binding site. Super-imposition of the antagonists was carried out using fit-atoms. This alignment was used to develop CoMFA models of the A2B antagonist binding site. The models possessed promising predictive ability as indicated by the high cross-validated correlation (q2 = 0.752, r2 = 0.982) and the prediction on the external test set. The analyses showed that steric and electrostatic interactions contributed to A2B antagonist biol. activity equally. The hydrogen-bond donor nature of the 7-position of xanthine (1 .apprx. 68) and 3-position of alloxazine (83) was essential for the biol. activity. In addition, the presence of more neg. charges on the 1-N position of xanthine and 10-N position of alloxazine increases biol. activity. The bulky aromatic substitutions on the 8-position of xanthine compds. improve activity, while an alkyl substitution on the 1-position of alloxazine might enhance activity. The model generated from this investigation produced important structural requirements, which will be used to optimize the structural complementarity of the antagonists at the A2B binding site.
IT **2398-70-1**, 6-Thiotheophylline **6603-63-0**
42458-91-3, 1-Methyl-3-isobutyl-6-thioxanthine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(structural predictions of adenosine 2B antagonist affinity using mol. field anal.)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 6603-63-0 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 42458-91-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

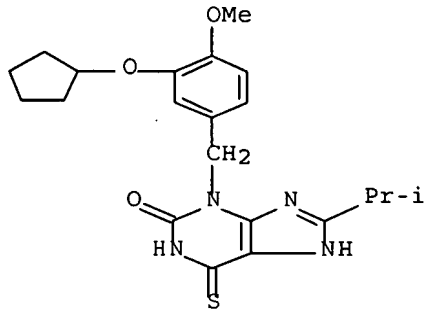
L57 ANSWER 7 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:413183 CAPLUS Full-text
DOCUMENT NUMBER: 135:164033
TITLE: An updated topographical model for phosphodiesterase 4 (PDE4) catalytic site
AUTHOR(S): Fossa, Paola; Menozzi, Giulia; Mosti, Luisa
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Genoa, 16132, Italy
SOURCE: Quantitative Structure-Activity Relationships (**2001**), 20(1), 17-22
CODEN: QSARDI; ISSN: 0931-8771
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 08 Jun 2001
AB Preclin. and clin. studies on cyclic nucleotide phosphodiesterases 4 (PDE4) inhibitors showed that these agents might be employed in the treatment of allergic diseases, in particular asthma. Unfortunately, many of these compds.

such as rolipram, which belongs to the so-called first generation" showed undesirable side effects such as nausea and emesis. Efforts to eliminate these adverse side effects prompted the synthesis of a second generation of PDE4 inhibitors, with improved selectivity toward the enzyme catalytic site. So as to refine the pharmacophoric models of the catalytic site previously described in literature and better define the structural requirements which are essential for potent and selective PDE4 inhibition, we undertook the present computational study. DISCO approach was applied to generate an optimal alignment for a set of structurally diverse selective inhibitors 1-18 chosen from the literature. The resulting superimposition of common pharmacophoric elements was refined by evaluating mol. field properties. A rational pharmacophoric model of the enzyme active site was thus derived and tested for its ability in predicting the degree of potency for a novel ligand. The comparison of the pharmacophoric areas common to cAMP, the natural substrate of the enzyme, and the most selective inhibitors was performed so as to better understand the binding mode of PDE4 selective inhibitors in the catalytic site.

IT **179486-28-3**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(updated topog. model for phosphodiesterase 4 (PDE4) catalytic site)

RN 179486-28-3 CAPLUS

CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)

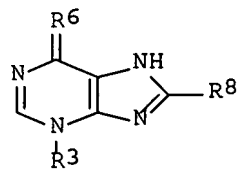


REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 8 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:136945 CAPLUS Full-text
DOCUMENT NUMBER: 134:193441
TITLE: Preparation of hypoxanthines and thiohypoxanthines as phosphodiesterase IV inhibitors
INVENTOR(S): Chasin, Mark; Hofer, Peter; Cavalla, David
PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2001011967 A1 20010222 WO 2000-US21836 20000809 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
CA 2379356 A1 20010222 CA 2000-2379356 20000809 <--
EP 1202628 A1 20020508 EP 2000-953925 20000809 <--
EP 1202628 B1 20041013
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL
JP 2003506467 T 20030218 JP 2001-516330 20000809 <--
AT 279113 T 20041015 AT 2000-953925 20000809 <--
PRIORITY APPLN. INFO.: US 1999-148623P P 19990812 <--
WO 2000-US21836 W 20000809 <--
OTHER SOURCE(S): MARPAT 134:193441
ED Entered STN: 25 Feb 2001
GI



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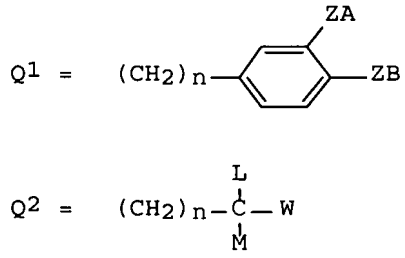
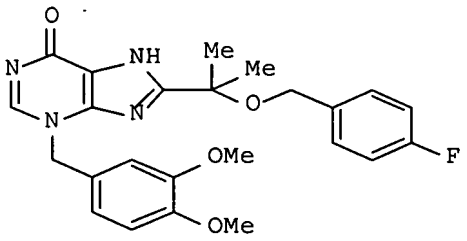




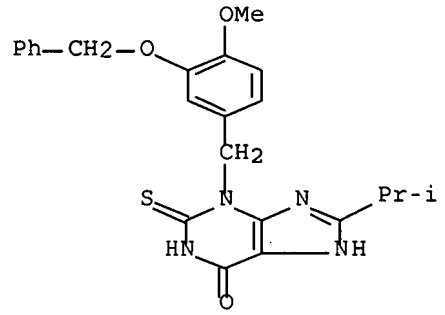
II

AB Title compds. (I) [wherein R3 and R8 = independently (cyclo)alkyl, alkenyl, alkynyl, Q1, or Q2; R6 = S or O; n = 0-1; Z = a bond, CH2, NH, O, or S; A and B can form a ring by adding 1-3 CH2 groups when Z = CH2, NH, O or S; and A and B are not in a ring when Z = a bond, wherein A and B = independently H, halo, (cyclo)alkyl, (cyclo)alkoxy, OH, or (un)substituted Ph, benzyl, or benzyloxy; L and M = independently H or Me; W = Q1, OH, (hetero)aryl, heterocyclyl, or (un)substituted benzyloxy] were prepared as selective phosphodiesterase (PDE) IV inhibitors. For example, amidation of 2-(4-fluorobenzyloxy)-2-methylpropionyl chloride with 5,6-diamino-1-(3,4-dimethoxybenzyl)-2-thiouracil using TEA in THF (20.4%), followed by cyclization with NaOH to form the 2-thioxanthine (79.1%) and treatment with Raney nickel in 1-propanol (67.2%), afforded the hypoxanthine (II). In assays measuring isolated PDE isoenzyme

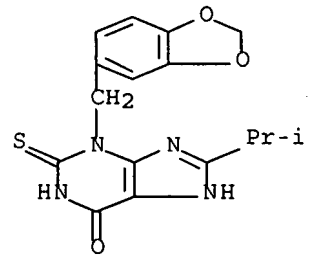
activity, II selectively inhibited PDE IV compared to PDE III and PDE V with IC50 values of 1.079 μM, 69.62 μM, and 35.80 μM, resp. As a result, I are expected to induce the desirable anti-asthmatic effects associated with PDE IV inhibition without causing the undesirable cardiovascular stimulation associated with PDE III inhibition (no data). I are useful in the treatment of asthma, allergies, inflammation, depression, dementia, and other disease states associated with abnormally high physiol. levels of cytokine (no data).

IT **227763-83-9P**, 3-(3-Benzyloxy-4-methoxybenzyl)-8-isopropyl-2-thioxanthine **327036-65-7P**, 3-(3,4-Methylenedioxybenzyl)-8-(1-methylethyl)-2-thioxanthine **327036-70-4P**, 3-(3,4-Dimethoxybenzyl)-8-(1-methylethyl)-2-thioxanthine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of hypoxanthine and thiohypoxanthine phosphodiesterase IV inhibitors from thiouracils and acyl halides and anhydrides)

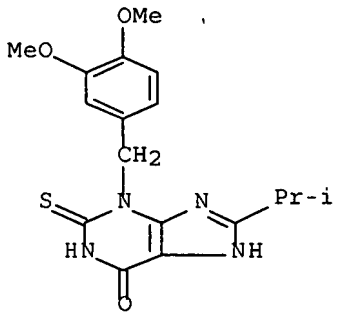
RN 227763-83-9 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



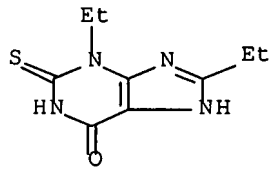
RN 327036-65-7 CAPLUS
CN 6H-Purin-6-one, 3-(1,3-benzodioxol-5-ylmethyl)-1,2,3,7-tetrahydro-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



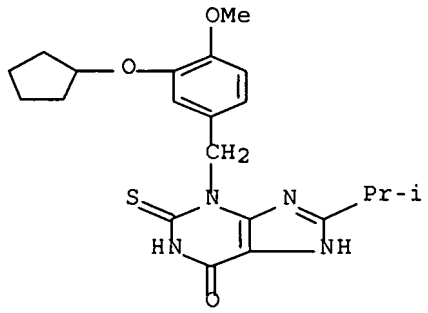
RN 327036-70-4 CAPLUS
CN 6H-Purin-6-one, 3-[(3,4-dimethoxyphenyl)methyl]-1,2,3,7-tetrahydro-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



IT **162278-04-8**, 3,8-Diethyl-2-thioxanthine **300781-30-0**, 3-(3-Cyclopentyloxy-4-methoxybenzyl)-8-isopropyl-2-thioxanthine
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of hypoxanthine and thiohypoxanthine phosphodiesterase IV inhibitors from thiouracils and acyl halides and anhydrides)
RN 162278-04-8 CAPLUS
CN 6H-Purin-6-one, 3,8-diethyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 300781-30-0 CAPLUS
CN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,2,3,7-tetrahydro-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 9 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:725418 CAPLUS Full-text
DOCUMENT NUMBER: 133:296324
TITLE: Synthesis and phosphodiesterase IV inhibition activity

of purine derivatives

INVENTOR(S): Chasin, Mark; Cavalla, David; Hofer, Peter; Gehrig, Andre; Wintergest, Peter

PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg

SOURCE: PCT Int. Appl., 112 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 21

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000059449	A2	20001012	WO 2000-US8525	20000331 <--
WO 2000059449	A3	20010104		
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
CA 2367143	A1	20001012	CA 2000-2367143	20000331 <--
EP 1169321	A2	20020109	EP 2000-919929	20000331 <--
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HU 200200938	A2	20021028	HU 2002-938	20000331 <--
JP 2002541078	T	20021203	JP 2000-609014	20000331 <--
BR 2000011182	A	20030610	BR 2000-11182	20000331 <--
JP 2001316314	A	20011113	JP 2000-136383	20000509 <--

PRIORITY APPLN. INFO.:	US 1999-285473	A	19990402 <--
	IN 1994-CA514	A1	19940630 <--
	WO 2000-US8525	W	20000331 <--

OTHER SOURCE(S): MARPAT 133:296324

ED Entered STN: 13 Oct 2000

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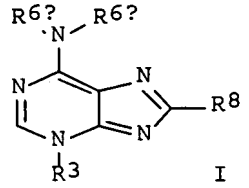

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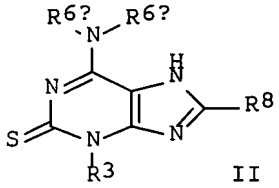

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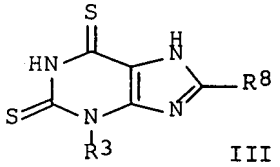

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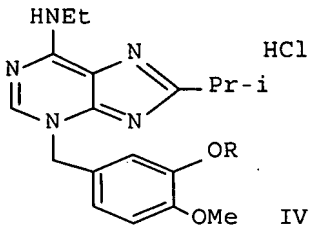

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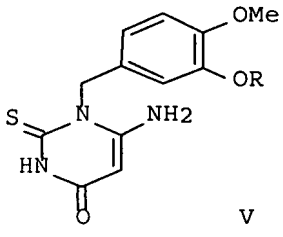

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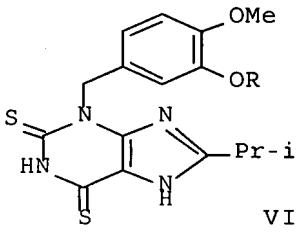
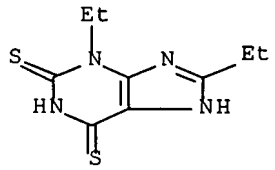


VI

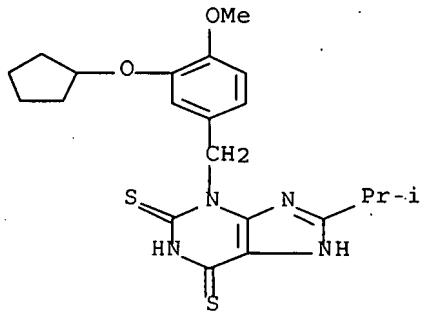
AB The purine (I) (R3, R8, R6a, R6b = H, (un)substituted alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, heteroaryl etc.), thioisoguanine (II), dithioxanthine (III) derivs., and their pharmaceutically accepted salts were synthesized. Thus, purine (IV; R = (CH2)5) was prepared by etherification of isovanilline with cyclopentanol, oximation, reduction to amine, conversion to isothiocyanate, amination to thiourea followed by heterocyclization with Et cyanoacetate to thiouracil (V). V was nitrosylated, reduced, reacted with isobutyric anhydride to give isobutyrylamine which on treatment with phosphorus pentasulfide gave dithioxanthine (VI). VI, in a pressure reactor gave purine-2-thione which was reduced with Raney-nickel to give IV. The IC50 of IV against phosphodiesterase IV inhibition was 0.32 μM. I, II and III were effective in effecting PDE IV inhibition in patients in need thereof.

IT **162278-92-4P**, 3,8-Diethyl-2,6-dithioxanthine **162279-04-1P** **162279-05-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of purine derivs. as phosphodiesterase IV inhibitors)

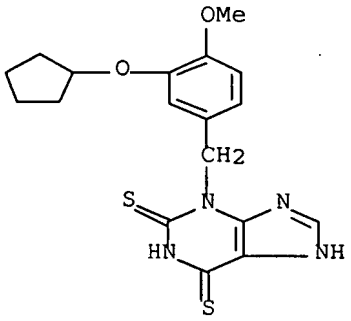
RN 162278-92-4 CAPLUS
CN 1H-Purine-2,6-dithione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162279-04-1 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)

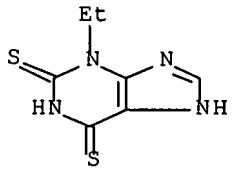


RN 162279-05-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro- (9CI) (CA INDEX NAME)

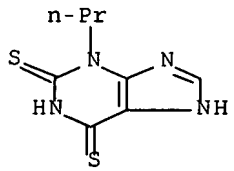


IT **162278-87-7P 162278-88-8P 162278-89-9P**
162278-90-2P 162278-91-3P 162278-93-5P
162278-94-6P 162279-01-8P 162279-02-9P
162279-06-3P 162279-07-4P 162279-08-5P
162279-09-6P 162279-10-9P 300783-45-3P
300783-48-6P 300783-53-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of purine derivs. as phosphodiesterase IV inhibitors)

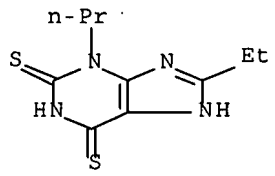
RN 162278-87-7 CAPLUS
CN 1H-Purine-2,6-dithione, 3-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



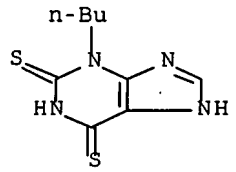
RN 162278-88-8 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-propyl- (9CI) (CA INDEX NAME)



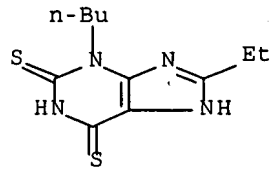
RN 162278-89-9 CAPLUS
CN 1H-Purine-2,6-dithione, 8-ethyl-3,7-dihydro-3-propyl- (9CI) (CA INDEX NAME)



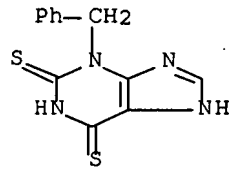
RN 162278-90-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3-butyl-3,7-dihydro- (9CI) (CA INDEX NAME)



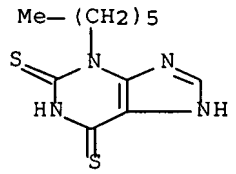
RN 162278-91-3 CAPLUS
CN 1H-Purine-2,6-dithione, 3-butyl-8-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



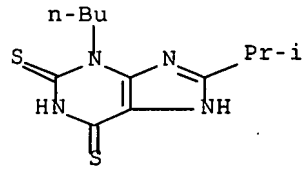
RN 162278-93-5 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



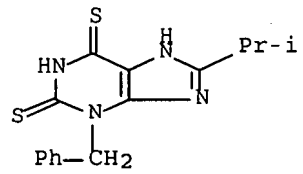
RN 162278-94-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3-hexyl-3,7-dihydro- (9CI) (CA INDEX NAME)



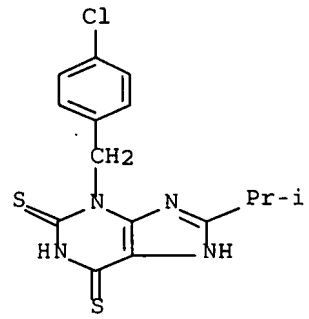
RN 162279-01-8 CAPLUS
CN 1H-Purine-2,6-dithione, 3-butyl-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



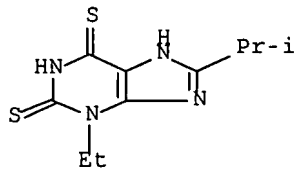
RN 162279-02-9 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



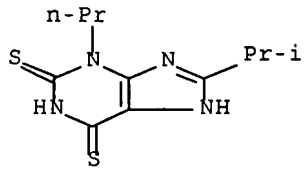
RN 162279-06-3 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[(4-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



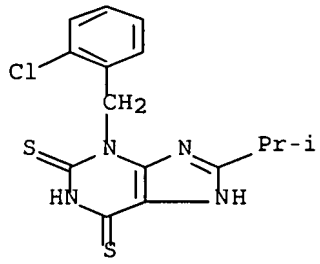
RN 162279-07-4 CAPLUS
CN 1H-Purine-2,6-dithione, 3-ethyl-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



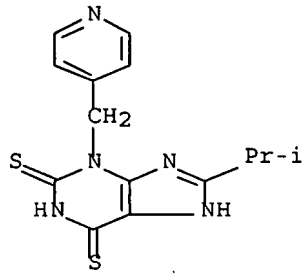
RN 162279-08-5 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-propyl- (9CI) (CA INDEX NAME)



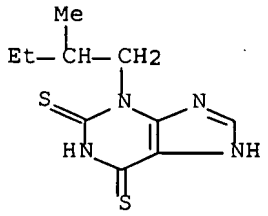
RN 162279-09-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[(2-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



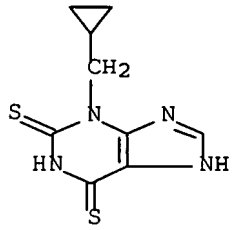
RN 162279-10-9 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



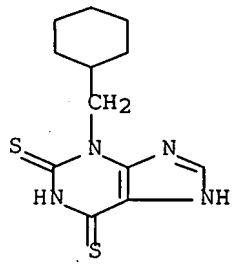
RN 300783-45-3 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-(2-methylbutyl)- (9CI) (CA INDEX NAME)



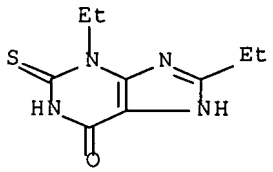
RN 300783-48-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3-(cyclopropylmethyl)-3,7-dihydro- (9CI) (CA INDEX NAME)



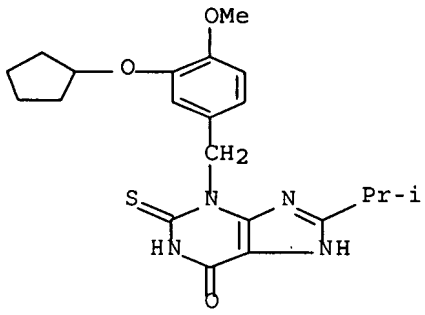
RN 300783-53-3 CAPLUS
CN 1H-Purine-2,6-dithione, 3-(cyclohexylmethyl)-3,7-dihydro- (9CI) (CA INDEX NAME)



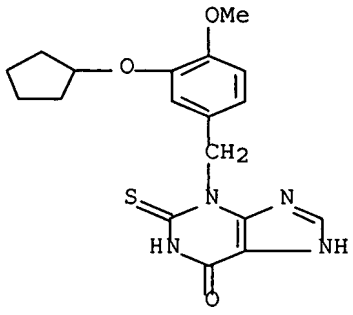
IT **162278-04-8**, 3,8-Diethyl-2-thioxanthine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of purine derivs. as phosphodiesterase IV inhibitors)
RN 162278-04-8 CAPLUS
CN 6H-Purin-6-one, 3,8-diethyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



IT **300781-30-0P 300781-35-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of purine derivs. as phosphodiesterase IV inhibitors)
RN 300781-30-0 CAPLUS
CN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,2,3,7-tetrahydro-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



RN 300781-35-5 CAPLUS
CN 6H-Purin-6-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



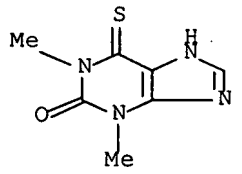
L57 ANSWER 10 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:721225 CAPLUS Full-text
DOCUMENT NUMBER: 134:28992
TITLE: Solvent-free synthesis of thio-alkylxanthines from alkylxanthines using microwave irradiation
AUTHOR(S): Rico-Gomez, Rodrigo; Najera, Francisco; Lopez-Romero, Juan Manuel; Canada-Rudner, Pedro
CORPORATE SOURCE: Departamento de Quimica Organica. Universidad de

Malaga, E-29071, Spain
SOURCE: Heterocycles (2000), 53(10), 2275-2278
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:28992
ED Entered STN: 13 Oct 2000

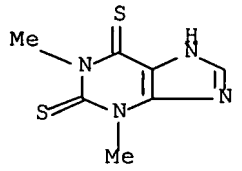
AB An expeditious, solvent-free procedure for the conversion of the xanthine bases theophylline, 8-methyltheophylline, caffeine, and theobromine to the corresponding 6-thio and 2,6-dithio derivs. using Lawesson's reagent under microwave irradiation is proposed.

IT **2398-70-1P**, 6-Thiotheophylline **6501-94-6P**
42459-09-6P 310904-66-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solvent-free synthesis of thioalkylxanthines from alkylxanthines using microwave irradiation)

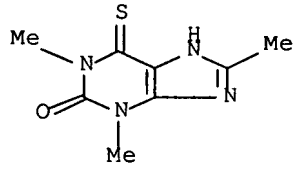
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 6501-94-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)

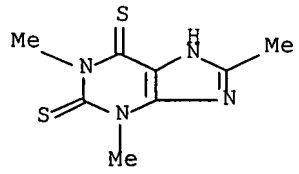


RN 42459-09-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3,8-trimethyl-6-thioxo- (9CI) (CA INDEX NAME)



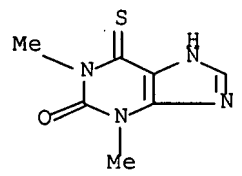
RN 310904-66-6 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3,8-trimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 11 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:544279 CAPLUS Full-text
DOCUMENT NUMBER: 133:281955
TITLE: New synthetic approach to theophylline and 6-thiotheophylline nucleosides from glycosyl derivatives of 4, 5-diaminouracil
AUTHOR(S): Rico-Gomez, Rodrigo; Lopez-Romero, Juan Manuel
CORPORATE SOURCE: Department de Quimica Organica, Facultad de Ciencias, Department de Quimica Organica, Facultad de Ciencias, Universidad de Malaga, Malaga, E-29071, Spain
SOURCE: Recent Research Developments in Organic & Bioorganic Chemistry (1999), 3, 93-106
CODEN: RDOBFG
PUBLISHER: Transworld Research Network
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
ED Entered STN: 09 Aug 2000
AB A review with 75 refs. on the syntheses of 7-theophylline nucleosides with special emphasis in the methods of construction of theophylline ring from 5-glycosylaminouracil. Preparation of 6-thiotheophylline nucleosides is also discussed.
IT **2398-70-1P**, 6-Thiotheophylline
RL: SPN (Synthetic preparation); PREP (Preparation)
(nucleoside derivs.; new synthetic approach to theophylline and thiotheophylline nucleosides from glycosyl derivs. of diaminouracil)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 113 THERE ARE 113 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

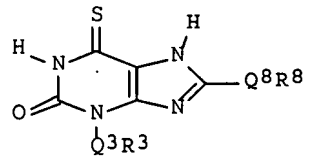
L57 ANSWER 12 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:344117 CAPLUS Full-text
DOCUMENT NUMBER: 132:347579
TITLE: Preparation of aryl thioxanthines as PDE IV inhibitors
INVENTOR(S): Cavalla, David; Hofer, Peter; Chasin, Mark
PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg
SOURCE: U.S., 12 pp., Cont.-in-part of U.S. Ser. No. 354,664, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 21
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6066641	A	20000523	US 1997-860680	19970611 <--
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
WO 9618399	A1	19960620	WO 1995-US16723	19951212 <--
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6440979	B1	20020827	US 2000-547898	20000412 <--

PRIORITY APPLN. INFO.:

US 1994-354664	B2	19941213 <--
WO 1995-US16723	W	19951212 <--
IN 1994-CA514	A1	19940630 <--
US 1997-860680	A1	19970611 <--

OTHER SOURCE(S): MARPAT 132:347579
ED Entered STN: 24 May 2000
GI



I

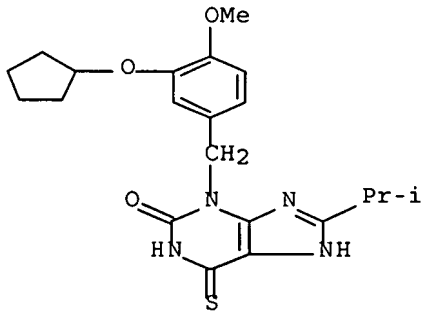
AB The title compds. [I; Q3 = a bond, alkylene, alkenylene, alkynylene; Q8 = alkylene, alkenylene, alkynylene; R3 = H, (un)substituted aryl, pyridyl, etc.; R8 = H, (un)substituted aryl, pyrimidinyl, etc.; provided that Q3R3 is not H or Me; and at least one of R3 and R8 = aryl, pyridyl, pyrimidinyl, quinolinyl or isoquinolinyl] which possess PDE-IV inhibitory activity and improved selectivity with regard to PDE-III inhibition, were prepared E.g., a multi-step synthesis of I [Q3R3 = 3-cyclopentyloxy-4- methoxybenzyl; Q8R8 = iso-Pr] which showed IC50 of 1.0 μM against PDE IV vs. IC50 of 2.8 μM against PDE IV for rolipram in the same assay, was given.

IT **179486-28-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of aryl thioxanthines as PDE IV inhibitors)

RN 179486-28-3 CAPLUS

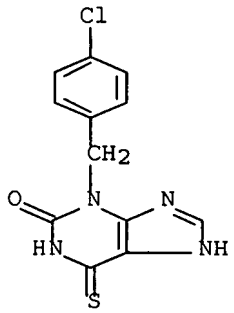
CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



IT **179486-29-4P 179486-30-7P 179486-31-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryl thioxanthines as PDE IV inhibitors)

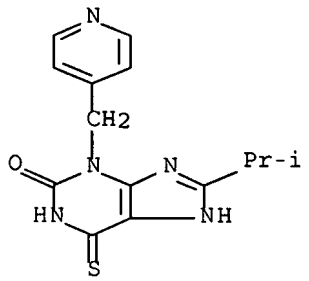
RN 179486-29-4 CAPLUS

CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)

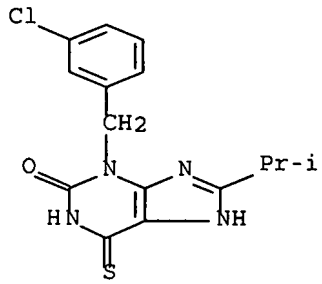


RN 179486-30-7 CAPLUS

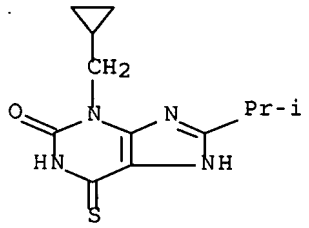
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-3-(4-pyridinylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



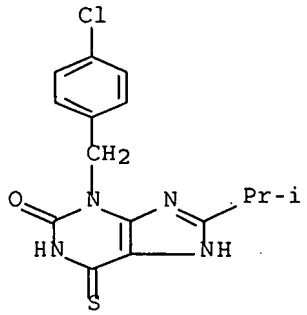
RN 179486-31-8 CAPLUS
CN 2H-Purin-2-one, 3-[(3-chlorophenyl)methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



IT **179486-64-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aryl thioxanthines as PDE IV inhibitors)
RN 179486-64-7 CAPLUS
CN 2H-Purin-2-one, 3-(cyclopropylmethyl)-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



IT **179486-60-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl thioxanthines as PDE IV inhibitors)
RN 179486-60-3 CAPLUS
CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)

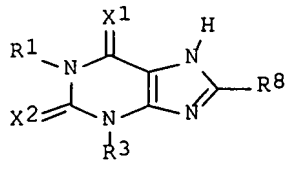


REFERENCE COUNT: 178 THERE ARE 178 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 13 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:113098 CAPLUS Full-text
DOCUMENT NUMBER: 132:151831
TITLE: Preparation of thioxanthines as PDE IV inhibitors
INVENTOR(S): Cavalla, David; Hofer, Peter; Chasin, Mark
PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg
SOURCE: U.S., 12 pp., Cont.-in-part of U.S. Ser. No. 476,262, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 21
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6025361	A	20000215	US 1997-860674	19970929 <--
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
CA 2206804	A1	19960620	CA 1995-2206804	19951212 <--
CA 2206804	C	20020319		
WO 9618400	A1	19960620	WO 1995-US16724	19951212 <--
W: AL, AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
IN 1995CA01665	A	20050304	IN 1995-CA1665	19951218 <--
US 5977119	A	19991102	US 1997-931849	19970915 <--
US 6268373	B1	20010731	US 1999-361196	19990726 <--
PRIORITY APPLN. INFO.:			US 1994-354664 B2	19941213 <--
			US 1995-476262 B2	19950607 <--
			WO 1995-US16724 W	19951212 <--
			IN 1994-CA514 A1	19940630 <--
			US 1997-860674 A1	19970929 <--

OTHER SOURCE(S): MARPAT 132:151831
ED Entered STN: 17 Feb 2000
GI



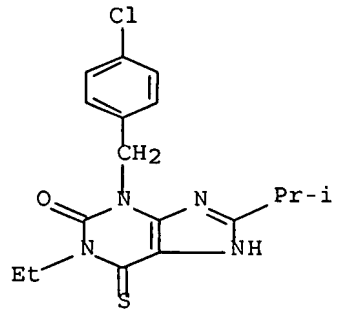
I

AB Title compds. [I; R1,R3,R8 = alkyl or aryl(alkyl); 1 of X1,X2 = S and the other = O or S] were prepared Thus, 5,6-diamino-1,3-diethyl-2-thiouracil was N-acylated by cyclopropanecarbonyl chloride and the cyclized product treated with P4S10 to give I (R1 = R3 = Et, X1 = X2 = S). Data for biol. activity of I were given.

IT **179951-27-0P 179951-29-2P 179951-30-5P**
179951-31-6P 179951-32-7P 179951-35-0P
179951-37-2P 179951-38-3P 179951-40-7P
179951-41-8P 257939-27-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thioxanthines as PDE IV inhibitors)

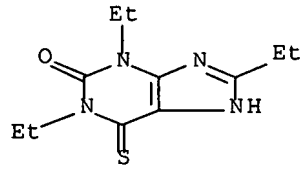
RN 179951-27-0 CAPLUS

CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1-ethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



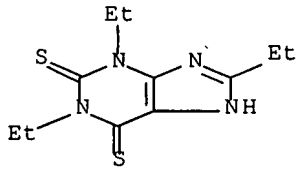
RN 179951-29-2 CAPLUS

CN 2H-Purin-2-one, 1,3,8-triethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)

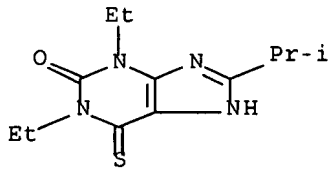


RN 179951-30-5 CAPLUS

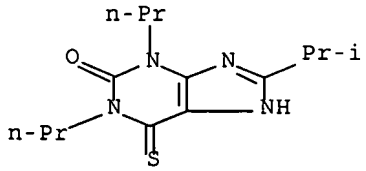
CN 1H-Purine-2,6-dithione, 1,3,8-triethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



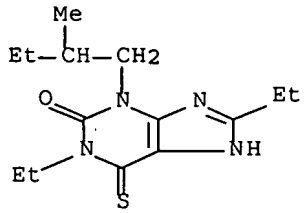
RN 179951-31-6 CAPLUS
CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



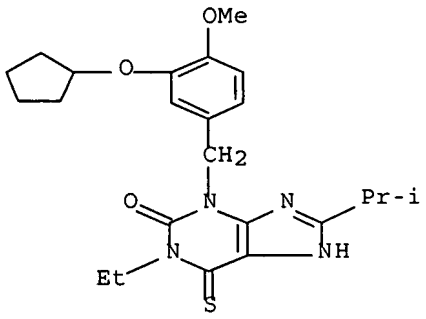
RN 179951-32-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



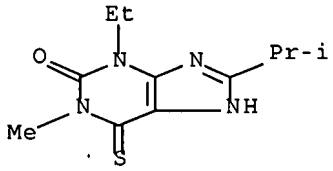
RN 179951-35-0 CAPLUS
CN 2H-Purin-2-one, 1,8-diethyl-1,3,6,7-tetrahydro-3-(2-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)



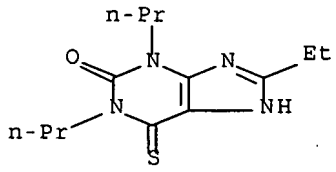
RN 179951-37-2 CAPLUS
CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1-ethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



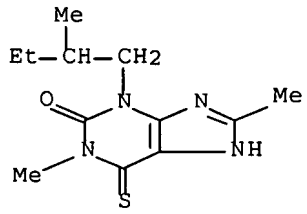
RN 179951-38-3 CAPLUS
CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-1-methyl-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



RN 179951-40-7 CAPLUS
CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)

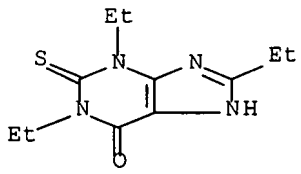


RN 179951-41-8 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,8-dimethyl-3-(2-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)



RN 257939-27-8 CAPLUS
CN 6H-Purin-6-one, 1,3,8-triethyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA

INDEX NAME)

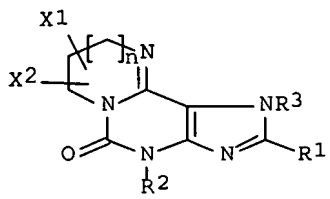


REFERENCE COUNT: 186 THERE ARE 186 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 14 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:34744 CAPLUS Full-text
DOCUMENT NUMBER: 132:88180
TITLE: Condensed purine derivatives as remedies for diabetes
INVENTOR(S): Shimada, Junichi; Ohta, Yoshihisa; Takasaki, Kotaro; Suda, Miho; Kusaka, Hideaki; Yano, Hiroshi; Nakanishi, Satoshi; Matsuda, Yuzuru
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000001388	A1	20000113	WO 1999-JP3583	19990702 <--
W: AU, BG, BR, CA, CN, CZ, HU, ID, IL, IN, JP, KR, MX, NO, NZ, PL, RO, SG, SI, SK, UA, US, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2336412	A1	20000113	CA 1999-2336412	19990702 <--
AU 9943968	A	20000124	AU 1999-43968	19990702 <--
EP 1092435	A1	20010418	EP 1999-926903	19990702 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 6489331	B1	20021203	US 2001-719570	20010409 <--
PRIORITY APPLN. INFO.:			JP 1998-187705 A	19980702 <--
			WO 1999-JP3583 W	19990702 <--

ED Entered STN: 14 Jan 2000
GI

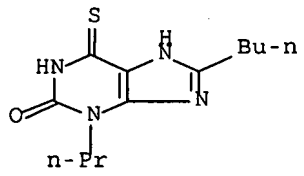


I

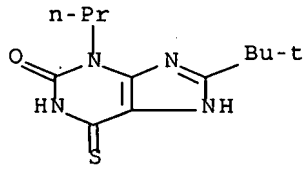
AB Remedies for diabetes which contain condensed purine derivs. as the active ingredient compds. represented by general formula (I) or physiol. acceptable salts thereof wherein R1 represents hydrogen, lower alkyl, optionally substituted aryl or optionally substituted heteroaryl; R2 represents hydrogen, lower alkyl, optionally substituted aralkyl, optionally substituted aryl or optionally substituted heteroaryl; R3 represents hydrogen, lower alkyl or optionally substituted aralkyl; X1 and X2 independently represent each hydrogen, lower alkyl, optionally substituted aralkyl or optionally substituted aryl; and n is an integer from 0 to 3. I can promote insulin secretion. Formulation examples of I were given.

IT **114834-11-6 254427-32-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensed purine derivs. as remedies for diabetes)

RN 114834-11-6 CAPLUS
CN 2H-Purin-2-one, 8-butyl-1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



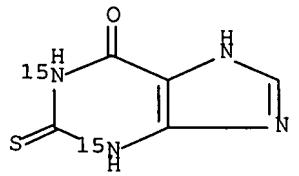
RN 254427-32-2 CAPLUS
CN 2H-Purin-2-one, 8-(1,1-dimethylethyl)-1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



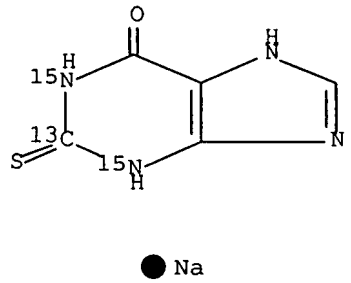
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 15 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:491591 CAPLUS Full-text
DOCUMENT NUMBER: 131:257779
TITLE: 15N-Multi-labeled Adenine and Guanine Nucleosides. Syntheses of [1,3,NH2-15N3]- and [2-13C-1,3,NH2-15N3]-Labeled Adenosine, Guanosine, 2'-Deoxyadenosine, and 2'-Deoxyguanosine
AUTHOR(S): Abad, Jose-Luis; Gaffney, Barbara L.; Jones, Roger A.
CORPORATE SOURCE: Department of Chemistry, Rutgers The State University of New Jersey, Piscataway, NJ, 08854, USA
SOURCE: Journal of Organic Chemistry (**1999**), 64(18), 6575-6582
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 10 Aug 1999
AB The authors report a high-yield route to the following specifically 15N- and 13C-multi-labeled nucleosides: [1,3,NH2-15N3]- and [2-13C-1,3,NH2-15N3]-adenosine; [1,3,NH2-15N3]- and [2-13C-1,3,NH2-15N3]- guanosine; [1,3,NH2-15N3]- and [2-13C-1,3,NH2-15N3]-2'-deoxyadenosine; [1,3,NH2-15N3]- and [2-13C-1,3,NH2-15N3]-2'-deoxyguanosine. In each set, the 13C2 atom functions as a "tag" that allows the 15N1 and 15N3 atoms to be unambiguously differentiated from the untagged versions in 15N NMR of RNA or DNA fragments. The key intermediate of this synthetic strategy for both the adenine and guanine nucleosides is [NH2,CONH2-15N2]-5-amino-4- imidazolecarboxamide. The [2-13C]-label is added through a ring closure using [13C]-sodium Et xanthate (NaS13CSOEt). Enzymic transglycosylation of either multi-labeled 6-chloropurine or multi-labeled 2-mercaptohypoxanthine and a final reaction with 15NH3 give the adenine and guanine nucleosides. This is the first report of a [3-15N]-labeled guanine nucleoside.
IT **244769-62-8P 244769-79-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(syntheses of [15N3]- and [13C,15N3]-labeled adenosine, guanosine, deoxyadenosine, and deoxyguanosine nucleosides)
RN 244769-62-8 CAPLUS
CN 6H-Purin-6-one-1,3-15N2, 1,2,3,7-tetrahydro-2-thioxo-, monosodium salt (9CI) (CA INDEX NAME)

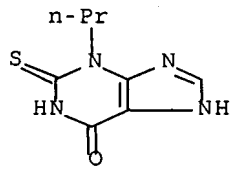


RN 244769-79-7 CAPLUS
CN 6H-Purin-6-one-2-13C-1,3-15N2, 1,2,3,7-tetrahydro-2-thioxo-, monosodium salt (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 16 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:412389 CAPLUS Full-text
DOCUMENT NUMBER: 131:179928
TITLE: 1,3-Dialkylxanthine derivatives having high potency as antagonists at human A2b adenosine receptors
AUTHOR(S): Jacobson, Kenneth A.; Ijzerman, Ad P.; Linden, Joel
CORPORATE SOURCE: Molecular Recognition Section, Laboratory of Bioorganic Chemistry, National Institute of Diabetes, Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD, 20892-0810, USA
SOURCE: Drug Development Research (**1999**), 47(1), 45-53
CODEN: DDREDK; ISSN: 0272-4391
PUBLISHER: Wiley-Liss, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 05 Jul 1999
AB The structure-activity relationships (SAR) of alkylxanthine derivs. as antagonists at the recombinant human adenosine receptors were explored in order to identify selective antagonists of A2B receptors. The effects of lengthening alkyl substituents from Me to Bu at 1- and 3-positions and addnl. substitution at the 7- and 8-positions were probed. Ki values, determined in competition binding in membranes of HEK-293 cells expressing A2B receptors using 125I-ABOPX (125I-3-(4-amino-3-iodobenzyl)-8-(phenyl-4- oxyacetate)-1-propylxanthin e), were approx. 10 to 100 nM for 8-phenylxanthine functionalized congeners. Xanthines containing 8-aryl, 8-alkyl, and 8-cycloalkyl substituents, derivs. of XCC (8-[4-[[[carboxy]methyl]oxy]phenyl]-1,3-dipropylxanthine) and XAC (8-[4-[[[[(2-amino-ethyl)amino]carbonyl]methyl]-oxy]phenyl]-1,3- dipropylxanthine), containing various ester and amide groups, including L- and D-amino acid conjugates, were included. Enprofylline was 2-fold more potent than theophylline in A2B receptor binding, and the 2-thio modification was not tolerated. Among the most potent derivs. examined were XCC, its hydrazide and aminoethyl and fluoroethyl amide derivs., XAC, N-hydroxyethyl-XAC, and the L-citrulline and D-p-aminophenylalanine conjugates of XAC. An N-hydroxysuccinimide ester of XCC (XCC-NHS, MRS 1204) bound to A2B receptors with a Ki of 9.75 nM and was the most selective (at least 20-fold) in this series. In a functional assay of recombinant human A2B receptors, four of these potent xanthines were shown to fully antagonize the effects of NECA-induced stimulation of cAMP accumulation.
IT **156733-29-8**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(1,3-Dialkylxanthine derivs. having high potency as antagonists at human A2b adenosine receptors)
RN 156733-29-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-propyl-2-thioxo- (9CI) (CA INDEX NAME)

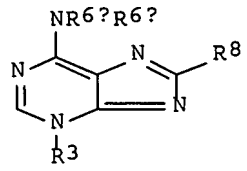


REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 17 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:404966 CAPLUS Full-text
DOCUMENT NUMBER: 131:58700
TITLE: Preparation of purine derivatives having phosphodiesterase IV inhibiting activity
INVENTOR(S): Cavalla, David; Chasin, Mark; Hofer, Peter; Gehrig, Andre; Wintergerst, Peter
PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg
SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 21
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 9931102	A1	19990624	WO 1998-US26293		19981211	<--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW						
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG						
IN 180930	A1	19980404	IN 1995-CA1508		19951123	<--
IN 181538	A1	19980711	IN 1995-CA1506		19951123	<--
US 6037470	A	20000314	US 1998-209658		19981210	<--
US 6040447	A	20000321	US 1998-209922		19981210	<--
US 6057445	A	20000502	US 1998-209664		19981210	<--
CA 2314335	A1	19990624	CA 1998-2314335		19981211	<--
AU 9918159	A	19990705	AU 1999-18159		19981211	<--
AU 747366	B2	20020516				
BR 9815171	A	20001010	BR 1998-15171		19981211	<--
EP 1045849	A1	20001025	EP 1998-963053		19981211	<--
EP 1045849	B1	20030702				
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI						
TR 200001706	T2	20001121	TR 2000-200001706		19981211	<--
US 6211367	B1	20010403	US 1998-210557		19981211	<--
US 6228859	B1	20010508	US 1998-210556		19981211	<--
HU 200100417	A2	20011228	HU 2001-417		19981211	<--
JP 2002508376	T	20020319	JP 2000-539025		19981211	<--
JP 3504234	B2	20040308				
AT 244243	T	20030715	AT 1998-963053		19981211	<--
PT 1045849	T	20031128	PT 1998-963053		19981211	<--
ES 2202924	T3	20040401	ES 1998-963053		19981211	<--
NO 2000002998	A	20000719	NO 2000-2998		20000609	<--
PRIORITY APPLN. INFO.:			US 1997-69371P	P	19971212	<--
			IN 1994-CA514	A1	19940630	<--
			WO 1998-US26293	W	19981211	<--

OTHER SOURCE(S): MARPAT 131:58700
ED Entered STN: 01 Jul 1999
GI



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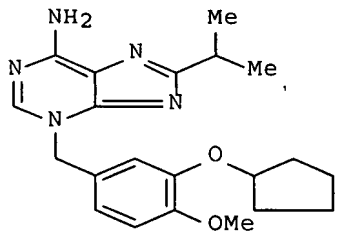


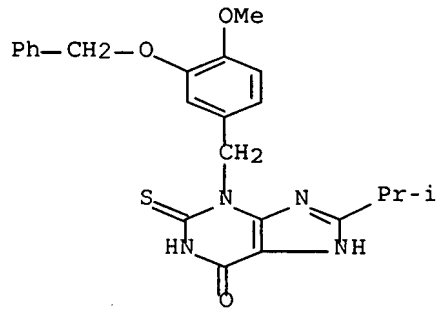
II

AB Purines I [R3 = alkyl, alkenyl, cycloalkyl, cycloalkenyl, wherein said alkyl, alkenyl, cycloalkyl, cycloalkylalkyl, cycloalkenyl; R6a, R6b = H, alkyl, alkenyl, cycloalkyl, cycloalkenyl; R8 = H, alkyl, alkenyl, cycloalkyl, cycloalkenyl] were prepared for use as phosphodiesterase inhibitors for the treatment of diseases such as asthma, allergy, or inflammation. Thus, purine derivative II was prepared starting from 3-(3-cyclopentyloxy-4-methoxybenzyl)-8-isopropylhypoxanthine. The prepared purines were tested for inhibitory activity against phosphodiesterase types III, IV, and V.

IT **227763-83-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of purine derivs. having phosphodiesterase IV inhibition activity)

RN 227763-83-9 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]-8-(1-methylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



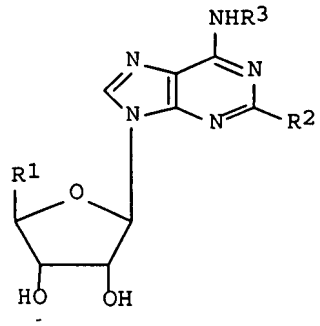
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 18 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:441960 CAPLUS Full-text
DOCUMENT NUMBER: 129:109311
TITLE: Preparation of nucleoside uronamides as A3 adenosine receptor agonists
INVENTOR(S): Jacobson, Kenneth A.; Gallo-Rodriguez, Carola; Van Galen, Philip J. M.; Von Lubitz, Dag K. J. E.; Jeong, Heaok Kim
PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, USA
SOURCE: U.S., 54 pp., Cont.-in-part of U. S. Ser. No. 163,324, abandoned.

CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
US 5773423	A	19980630	US 1994-274628		19940713	<--
US 5688774	A	19971118	US 1995-396111		19950228	<--
PRIORITY APPLN. INFO.:			US 1993-91109	B2	19930713	<--
			US 1993-163324	B2	19931206	<--
			US 1994-274628	A2	19940713	<--

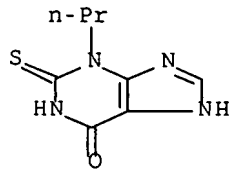
OTHER SOURCE(S): MARPAT 129:109311
ED Entered STN: 17 Jul 1998
GI



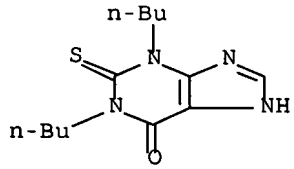
I

AB The present invention provides N6-benzyladenosine-5'-N-uronamide and related substituted compds. I (R1 = amide; R2 = halo, amino, alkenyl, alkynyl, thio, alkylthio; R3 = S-1-phenylethyl, Bn, phenylethyl), particularly those containing substituents on the benzyl and/or uronamide groups, and modified xanthine ribosides, as well as pharmaceutical compns. containing such compds. The present invention also provides a method of selectively activating an A3 adenosine receptor in a mammal, which method comprises acutely or chronically administering to a mammal in need of selective activation of its A3 adenosine receptor a therapeutically effective amount of a compound which binds with the A3 receptor so as to stimulate an A3 receptor-dependent response. Thus, N6-(3- iodobenzyl)adenosine was prepared tested for its affinity in binding at rat brain A1, A2, A3 adenosine receptors (Ki = 9.5-220.0 nM).

IT **156733-29-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nucleoside uronamides as A3 adenosine receptor agonists)
RN 156733-29-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-propyl-2-thioxo- (9CI) (CA INDEX NAME)



IT **77038-96-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of nucleoside uronamides as A3 adenosine receptor agonists)
RN 77038-96-1 CAPLUS
CN 6H-Purin-6-one, 1,3-dibutyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)

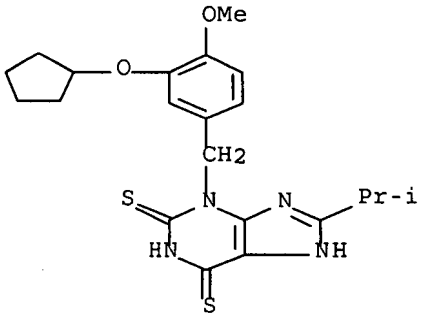


REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

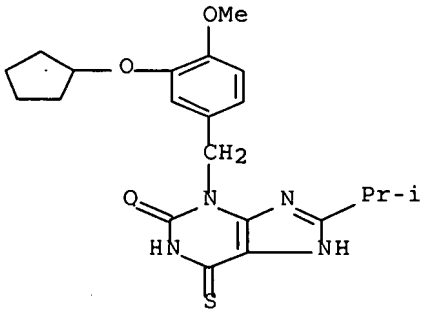
L57 ANSWER 19 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:153640 CAPLUS Full-text
DOCUMENT NUMBER: 128:303616
TITLE: Correlations of PDE-4 inhibition between enzymes of smooth muscle and inflammatory cell sources
AUTHOR(S): Cariuk, Peter; Cavalla, David; Chasin, Mark; Giembycz, Mark
CORPORATE SOURCE: Napp Research Centre, Cambridge Science Park, Cambridge, CB4 4GW, UK
SOURCE: Cell Biochemistry and Biophysics (1998), 28(2-3), 219-249
CODEN: CBBIFV; ISSN: 1085-9195
PUBLISHER: Humana Press Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 14 Mar 1998
AB The sensitivities of PDE-4 enzymes from smooth muscle and inflammatory cell sources from different species to a range of structurally diverse compds. were compared. All inflammatory cell PDE-4 sources displayed good cross-correlations in their sensitivity to inhibition by these compds. Similarly, PDE-4 enzymes from smooth muscle sources were well-correlated; however, there was no cross-correlation between PDE-4 from smooth muscle sources and those of inflammatory cell sources, possibly reflecting differences in subcellular location of enzymes as well as subtype expression. The present study concludes that PDE-4 prepns. from smooth muscle sources as well as those from inflammatory cell sources can be used to model the potential smooth muscle cell relaxing properties and antiinflammatory properties of a compound in relation to human asthma.
IT **162279-04-1 179486-28-3 179486-64-7**
179951-31-6 179951-32-7 179951-37-2

179951-38-3 206352-05-8 206352-07-0
206352-09-2 206352-16-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(correlations of PDE-4 inhibition between enzymes of smooth muscle and inflammatory cell sources)

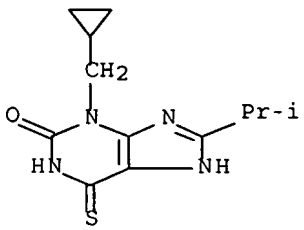
RN 162279-04-1 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



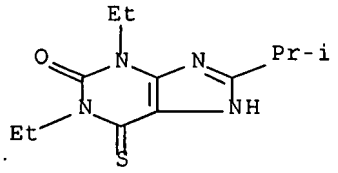
RN 179486-28-3 CAPLUS
CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



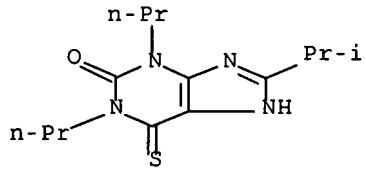
RN 179486-64-7 CAPLUS
CN 2H-Purin-2-one, 3-(cyclopropylmethyl)-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



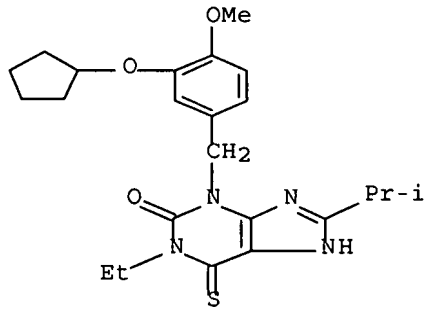
RN 179951-31-6 CAPLUS
CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



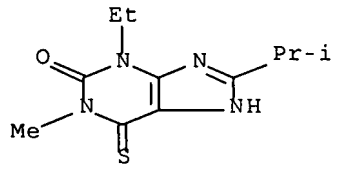
RN 179951-32-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



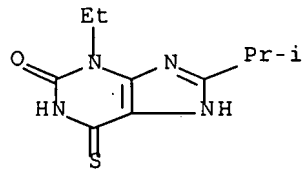
RN 179951-37-2 CAPLUS
CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1-ethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



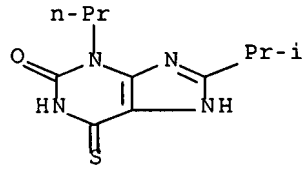
RN 179951-38-3 CAPLUS
CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-1-methyl-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



RN 206352-05-8 CAPLUS
CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



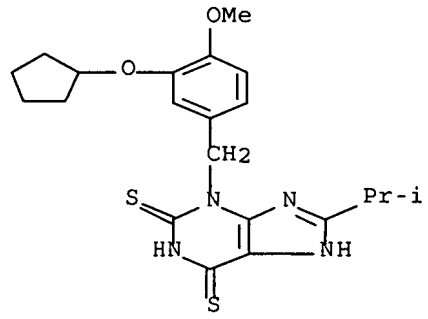
RN 206352-07-0 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 206352-09-2 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)-1H-purine-2,6-dithione (1:1) (9CI) (CA INDEX NAME)

CM 1

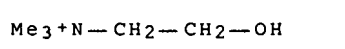
CRN 162279-04-1
CMF C21 H26 N4 O2 S2



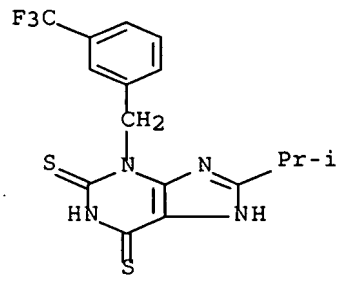
CM 2

CRN 62-49-7

CMF C5 H14 N O



RN 206352-16-1 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

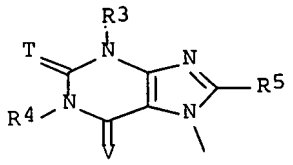


REFERENCE COUNT: 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L57 ANSWER 20 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:331961 CAPLUS Full-text
DOCUMENT NUMBER: 126:305588
TITLE: Preparation of 4-(dioxopurinylmethyl)phenylacetates and analogs as hypolipemics
INVENTOR(S): Connell, Richard; Goldmann, Siegfried; Mueller, Ulrich; Lohmer, Stefan; Bischoff, Hilmar; Denzer, Dirk; Gruetzmann, Rudi; Wohlfeil, Stefan
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Eur. Pat. Appl., 69 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 764647	A1	19970326	EP 1996-114577	19960912 <--
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
DE 19535504	A1	19970327	DE 1995-19535504	19950925 <--
US 5714494	A	19980203	US 1996-710503	19960918 <--
JP 09216884	A	19970819	JP 1996-267691	19960919 <--
CA 2186086	A1	19970326	CA 1996-2186086	19960920 <--

PRIORITY APPLN. INFO.: DE 1995-19535504 A 19950925 <--
OTHER SOURCE(S): MARPAT 126:305588
ED Entered STN: 24 May 1997
GI



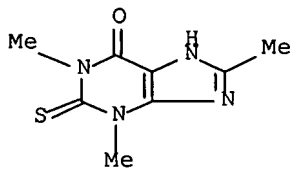
II

AB RCH2ZCHR1C(:L)R2 [I; R = xanthine moiety, e.g., II; R1 = H, (cyclo)alkyl, Ph, heterocyclyl, etc.; R2 = OH, SH, alkoxy, (di)alkylamino, etc.; R3,R4 = H, alkyl, aryl, etc.; R5 = H, halo, alkyl, aryl, etc.; L,T,V = O or S; Z = (un)substituted 1,4-phenylene] were prepared Thus, 5,6-diamino-1,3-dimethyluracil was cyclocondensed with 4-MeC6H4CHO and the product N-alkylated by 4-(BrCH2)C6H4CHR1CO2CMe3 (R1 = cyclopentyl)(preparation given) to give 4-(RCH2)C6H4CHR1CO2CMe3 (R = II, R1 = cyclopentyl, R3 = R4 = Me, R5 = C6H4Me-4, T = V = O). Data for biol. activity of I were given.

IT **19673-55-3P 189215-37-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 4-(dioxopurinylmethyl)phenylacetates and analogs as hypolipemics)

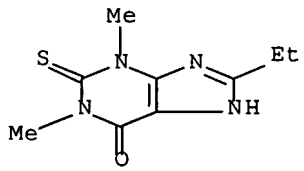
RN 19673-55-3 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3,8-trimethyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 189215-37-0 CAPLUS

CN 6H-Purin-6-one, 8-ethyl-1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 21 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:497159 CAPLUS Full-text

DOCUMENT NUMBER: 125:142465

TITLE: Preparation of 1,3,8-trialkylthioxoxanthines as phosphodiesterase inhibitors

INVENTOR(S): Cavalla, David J.; Hofer, Peter; Chasin, Mark

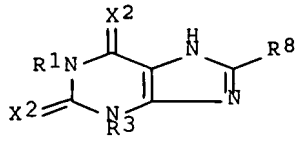
PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg

SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 21
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9618400	A1	19960620	WO 1995-US16724	19951212 <--
W: AL, AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
AU 9645279	A	19960703	AU 1996-45279	19951212 <--
EP 799040	A1	19971008	EP 1995-943950	19951212 <--
EP 799040	B1	20030820		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
JP 2001523213	T	20011120	JP 1996-519327	19951212 <--
AT 247655	T	20030915	AT 1995-943950	19951212 <--
US 6025361	A	20000215	US 1997-860674	19970929 <--
US 6268373	B1	20010731	US 1999-361196	19990726 <--

PRIORITY APPLN. INFO.:
US 1995-476262 A 19950607 <--
IN 1994-CA514 A1 19940630 <--
US 1994-354664 A 19941213 <--
WO 1995-US16724 W 19951212 <--
US 1997-860674 A1 19970929 <--

OTHER SOURCE(S): MARPAT 125:142465
ED Entered STN: 21 Aug 1996
GI



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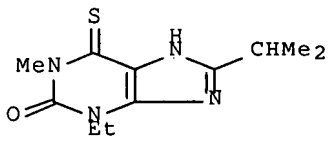
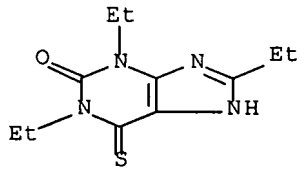


II

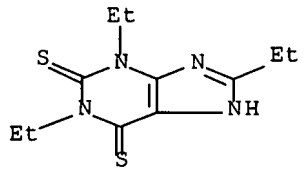
AB Title compds. [I; R1,R3,R8 = (ar)alkyl, aryl; 1 of X1,X2 = S and the other = O or S] were prepared Thus, title compound II had IC50 of 1.0μM against phosphodiesterase IV and V in vitro.

IT **179951-29-2P 179951-30-5P 179951-31-6P**
179951-32-7P 179951-35-0P 179951-37-2P
179951-38-3P 179951-40-7P 179951-41-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,3,8-trialkylthioxoxanthines as phosphodiesterase inhibitors)

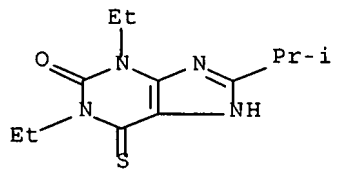
RN 179951-29-2 CAPLUS
CN 2H-Purin-2-one, 1,3,8-triethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



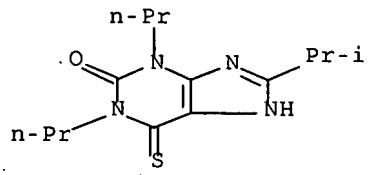
RN 179951-30-5 CAPLUS
CN 1H-Purine-2,6-dithione, 1,3,8-triethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



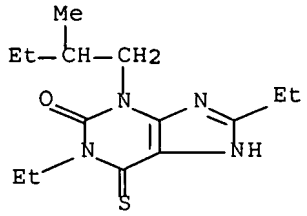
RN 179951-31-6 CAPLUS
CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



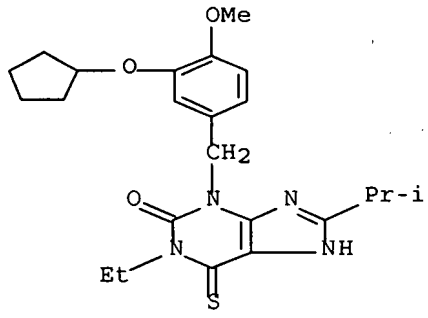
RN 179951-32-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



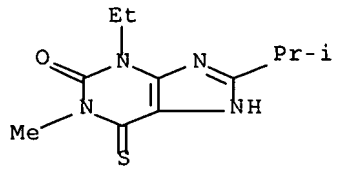
RN 179951-35-0 CAPLUS
CN 2H-Purin-2-one, 1,8-diethyl-1,3,6,7-tetrahydro-3-(2-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)



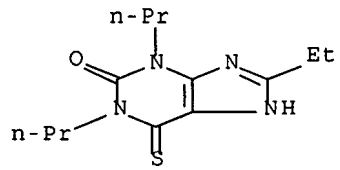
RN 179951-37-2 CAPLUS
CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1-ethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



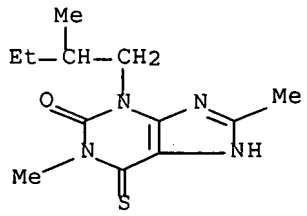
RN 179951-38-3 CAPLUS
CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-1-methyl-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



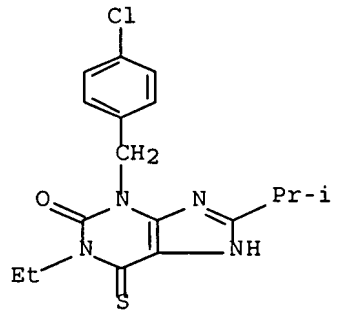
RN 179951-40-7 CAPLUS
CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 179951-41-8 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,8-dimethyl-3-(2-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)



IT **179951-27-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,3,8-trialkylthioxoxanthines as phosphodiesterase inhibitors)
RN 179951-27-0 CAPLUS
CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1-ethyl-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 22 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:473245 CAPLUS Full-text
DOCUMENT NUMBER: 125:142764
TITLE: Preparation of aryl thioxanthines as phosphodiesterase inhibitors
INVENTOR(S): Cavalla, David J.; Hofer, Peter; Chasin, Mark
PATENT ASSIGNEE(S): Euro-Celtique, S.A., Luxembourg
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 21
PATENT INFORMATION:

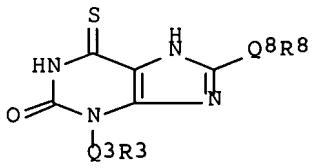
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9618399	A1	19960620	WO 1995-US16723	19951212 <--

W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ,

TM, TT
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

IN 180930	A1	19980404	IN 1995-CA1508		19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506		19951123 <--
CA 2206287	A1	19960620	CA 1995-2206287		19951212 <--
CA 2206287	C	20010320			
AU 9645278	A	19960703	AU 1996-45278		19951212 <--
EP 814809	A1	19980107	EP 1995-943949		19951212 <--
EP 814809	B1	20030813			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE					
JP 10508032	T	19980804	JP 1995-519326		19951212 <--
AT 247116	T	20030815	AT 1995-943949		19951212 <--
ZA 9510594	A	19960619	ZA 1995-10594		19951213 <--
ZA 9510595	A	19960619	ZA 1995-10595		19951213 <--
IN 1995CA01664	A	20050304	IN 1995-CA1664		19951218 <--
US 6066641	A	20000523	US 1997-860680		19970611 <--
US 6090816	A	20000718	US 1997-911549		19970814 <--
US 6440979	B1	20020827	US 2000-547898		20000412 <--
PRIORITY APPLN. INFO.:			US 1994-354664	A	19941213 <--
			IN 1994-CA514	A1	19940630 <--
			WO 1995-US16723	W	19951212 <--
			US 1997-860680	A1	19970611 <--

OTHER SOURCE(S): MARPAT 125:142764
ED Entered STN: 10 Aug 1996
GI



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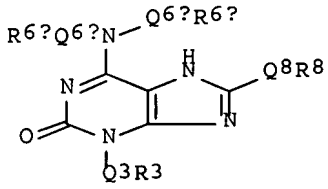


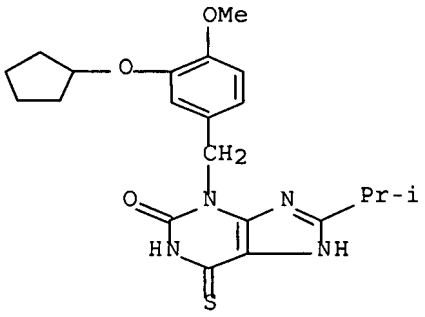
II

AB Title compds. I or II (Q3, Q6a, Q6b, Q8 are independently a bond, C1-8 alkylene, C2-8 alkenylene, C2-8 alkynylene; R3, R6a, R6b and R8 are independently H, aryl, heteroaryl, optionally substituted by halogen, hydroxy, alkoxy, nitro, cyano and carboxy, provided that Q3R3 is not H or Me in I or II, and at least one of R3 and R8 is aryl or heteroaryl in I), useful as phosphodiesterase inhibitors, are claimed. The compds. are effective PDE IV inhibitors and possess improved PDE IV inhibition and improved selectivity with regard to PDE III inhibition. Thus, the IC50 for 3-(3-cyclopentyloxy-4-methoxybenzyl)-8-isopropyl-6-thioxanthine (preparation given) was 1.0 μM for PDE IV inhibition, compared with 2.8 μM for rolipram.

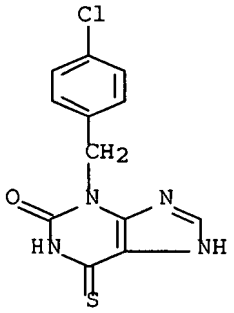
IT **179486-28-3P 179486-29-4P 179486-30-7P**
179486-31-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryl thioxanthines as phosphodiesterase inhibitors)

RN 179486-28-3 CAPLUS

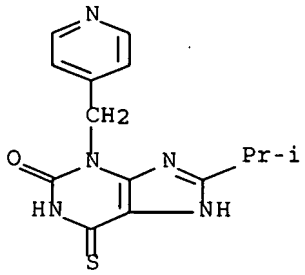
CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



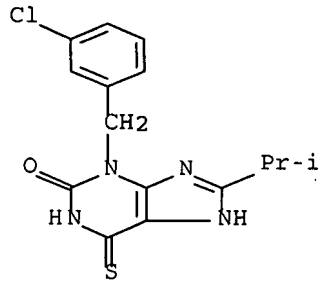
RN 179486-29-4 CAPLUS
CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



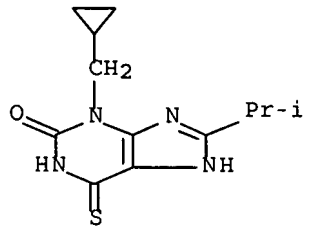
RN 179486-30-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-(1-methylethyl)-3-(4-pyridinylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



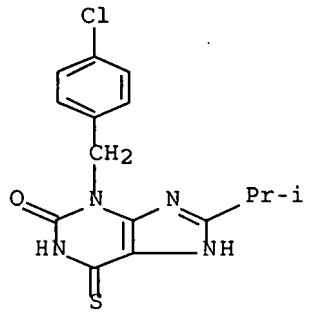
RN 179486-31-8 CAPLUS
CN 2H-Purin-2-one, 3-[(3-chlorophenyl)methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



IT **179486-64-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aryl thioxanthines as phosphodiesterase inhibitors)
RN 179486-64-7 CAPLUS
CN 2H-Purin-2-one, 3-(cyclopropylmethyl)-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)

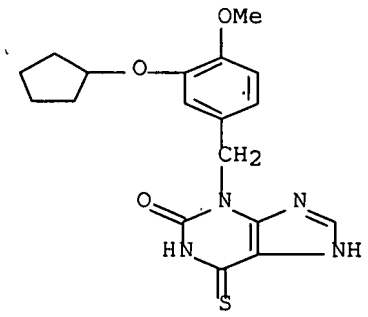


IT **179486-60-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl thioxanthines as phosphodiesterase inhibitors)
RN 179486-60-3 CAPLUS
CN 2H-Purin-2-one, 3-[(4-chlorophenyl)methyl]-1,3,6,7-tetrahydro-8-(1-methylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



IT **179486-67-0**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of aryl thioxanthines as phosphodiesterase inhibitors)
RN 179486-67-0 CAPLUS
CN 2H-Purin-2-one, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-1,3,6,7-

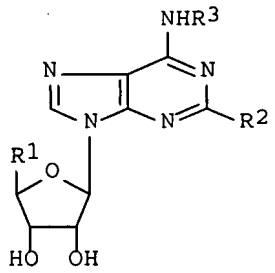
tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 23 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:837438 CAPLUS Full-text
DOCUMENT NUMBER: 123:257265
TITLE: Preparation of N6-benzyladenosine-5'-uronamides, modified xanthine ribosides, and related compounds as adenosine A3 receptor agonists.
INVENTOR(S): Jacobson, Kenneth A.; Gallo-Rodriguez, Carola; Von Galen, Philip J. M.; Von Lubitz, Dag K. J. E.; Jeong, Heaok Kim
PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, USA
SOURCE: PCT Int. Appl., 175 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9502604	A1	19950126	WO 1994-US7835		19940713 <--
W: AU, CA, JP					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
AU 9473310	A	19950213	AU 1994-73310		19940713 <--
EP 708781	A1	19960501	EP 1994-923445		19940713 <--
EP 708781	B1	20011004			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE					
AT 206432	T	20011015	AT 1994-923445		19940713 <--
PRIORITY APPLN. INFO.:			US 1993-91109	A	19930713 <--
			US 1993-163324	A	19931206 <--
			WO 1994-US7835	W	19940713 <--

OTHER SOURCE(S): MARPAT 123:257265
ED Entered STN: 07 Oct 1995
GI



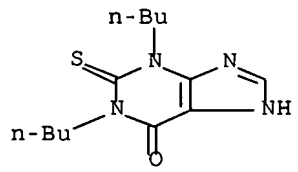
I

AB Title compds. [I; R1 = RaRbNCO, HORc; Ra, Rb = H, alkyl, amino, haloalkyl, aminoalkyl, cycloalkyl, BOC-aminoalkyl; RaRbN = heterocyclyl; Rc = alkyl, amino, haloalkyl, aminoalkyl, cycloalkyl, BOC-aminoalkyl; R2 = H, halo, alkyl ether residue, amino, alkylamino, alkenyl, alkynyl, thio, alkylthio; R3 = (R)- and (S)-1-phenylethyl, (substituted) PhCH2, substituted phenylethyl] and related compds., were prepared Thus, 2-chloro-N6-(3- iodobenzyl)adenine was refluxed with hexamethyldisilazane and cat. (NH4)2SO4 to give a silyl derivative which was refluxed with N-Me I-O-acetyl-2,3-dibenzoyl-α,β-D-ribofuronamide and trimethylsilyl triflate in dichloroethane to give 2-chloro-N6-(3- iodobenzyl)-9-[5-(methylamido)-2,3-di-O-benzoyl-β-D-ribofuranosyl]adenine. The latter was stirred with NH3 in MeOH for 16 h to give 68.7% 2-chloro-N6-(3-iodobenzyl)-9-[5-(methylamido)-β-D-ribofuranosyl]adenine. This showed Ki = 0.23 nM in a radioligand binding assay at rat brain A3 receptors.

IT **77038-96-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of N6-benzyladenosine-5'-uronamides, modified xanthine ribosides, and related compds. as adenosine A3 receptor agonists)

RN 77038-96-1 CAPLUS

CN 6H-Purin-6-one, 1,3-dibutyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 24 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:492020 CAPLUS Full-text

DOCUMENT NUMBER: 122:239459

TITLE: Preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors

INVENTOR(S): Cavalla, David; Hofer, Peter; Gehrig, Anddre; Wintergest, Peter

PATENT ASSIGNEE(S): Euro-Celtique S.A., Luxembourg

SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 21
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9500516	A1	19950105	WO 1994-GB1334	19940621 <--
W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2165433	A1	19941223	CA 1994-2165433	19940621 <--
CA 2165433	C	20020528		
AU 9469771	A	19950117	AU 1994-69771	19940621 <--
AU 683270	B2	19971106		
EP 705265	A1	19960410	EP 1994-918456	19940621 <--
EP 705265	B1	19990728		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1125445	A	19960626	CN 1994-192521	19940621 <--
CN 1045778	B	19991020		
HU 74176	A2	19961128	HU 1995-3545	19940621 <--
JP 09500376	T	19970114	JP 1995-502570	19940621 <--
JP 3350550	B2	20021125		
EP 916672	A1	19990519	EP 1999-100735	19940621 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
EP 916673	A1	19990519	EP 1999-100736	19940621 <--
EP 916673	B1	20030129		
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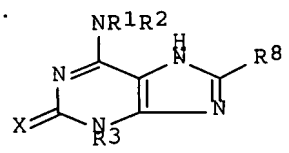
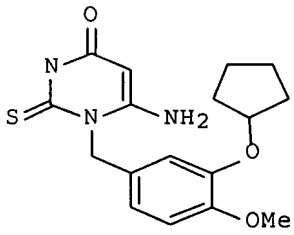
AT 182593	T	19990815	AT 1994-918456	19940621 <--
ES 2137371	T3	19991216	ES 1994-918456	19940621 <--
NZ 328914	A	20000825	NZ 1994-328914	19940621 <--
AT 231863	T	20030215	AT 1999-100736	19940621 <--
ZA 9404463	A	19950217	ZA 1994-4463	19940622 <--
IN 177888	A1	19970222	IN 1994-CA514	19940630 <--
TW 418208	B	20010111	TW 1994-83107047	19940802 <--
IN 180930	A1	19980404	IN 1995-CA1508	19951123 <--
IN 181538	A1	19980711	IN 1995-CA1506	19951123 <--
FI 9506168	A	19960201	FI 1995-6168	19951221 <--
NO 9505219	A	19960222	NO 1995-5219	19951221 <--
BG 62933	B1	20001130	BG 1995-100258	19951227 <--
US 5939422	A	19990817	US 1996-578580	19960408 <--
US 6310205	B1	20011030	US 1999-237638	19990126 <--
US 6294541	B1	20010925	US 1999-418330	19991014 <--
US 6319928	B1	20011120	US 1999-418331	19991014 <--

PRIORITY APPLN. INFO.:			
GB 1993-12853	A	19930622	<--
EP 1994-918456	A3	19940621	<--
NZ 1994-267468	A1	19940621	<--
WO 1994-GB1334	W	19940621	<--
IN 1994-CA514	A1	19940630	<--
US 1996-578580	A2	19960408	<--
US 1996-659767	A1	19960606	<--
US 1997-69371P	P	19971212	<--
US 1998-200615	B2	19981130	<--
US 1998-210556	A2	19981211	<--
US 1999-285473	A1	19990402	<--

OTHER SOURCE(S): MARPAT 122:239459
ED Entered STN: 18 Apr 1995
GI



I

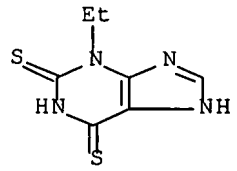


II

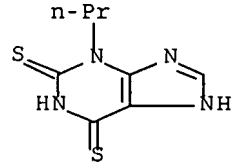
AB Title compds. [e.g., I; R1-R3,R8 = H, (cyclo)alkyl, (hetero)aryl, etc.; NR1R2 = heterocyclyl] were prepared Title compds. have bronchial and tracheal relaxation and/or antiinflammatory activity. Thus, isovanillin was converted in 5 steps to 3,4-(HO)(MeO)C6H3CH2NHCSNH2 which was cyclocondensed with NCCH2CO2Et to give thiouracil II. The latter was converted in 3 steps to 6-amino-1-(3-cyclopentyloxy-4-methoxybenzyl)-5- isobutyrylamino-2-thiouracil which was cyclized and the product converted in 4 steps to I.HCl (R1 = Et, R2 = H, R3 = 3-cyclopentyloxy-4- methoxybenzyl, R8 = CHMe2)(III). III gave 64% inhibition of ovalbumin-induced bronchoalveolar eosinophil production in guinea pigs at 5mg/kg i.p.

IT **162278-87-7P 162278-88-8P 162278-89-9P**
162278-90-2P 162278-91-3P 162278-93-5P
162278-94-6P 162279-01-8P 162279-02-9P
162279-04-1P 162279-05-2P 162279-06-3P
162279-07-4P 162279-08-5P 162279-09-6P
162279-10-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)

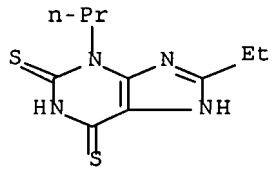
RN 162278-87-7 CAPLUS
CN 1H-Purine-2,6-dithione, 3-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



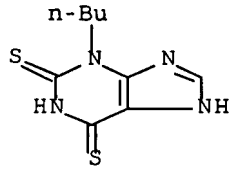
RN 162278-88-8 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-propyl- (9CI) (CA INDEX NAME)



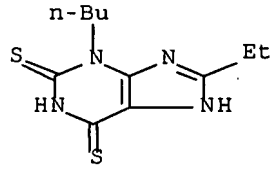
RN 162278-89-9 CAPLUS
CN 1H-Purine-2,6-dithione, 8-ethyl-3,7-dihydro-3-propyl- (9CI) (CA INDEX NAME)



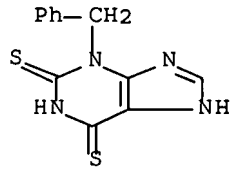
RN 162278-90-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3-butyl-3,7-dihydro- (9CI) (CA INDEX NAME)



RN 162278-91-3 CAPLUS
CN 1H-Purine-2,6-dithione, 3-butyl-8-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)

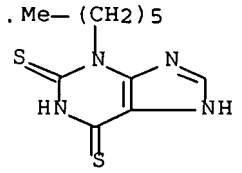


RN 162278-93-5 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

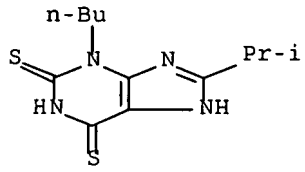


RN 162278-94-6 CAPLUS

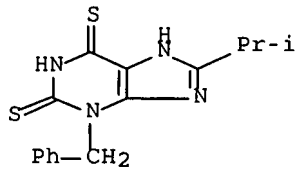
CN 1H-Purine-2,6-dithione, 3-hexyl-3,7-dihydro- (9CI) (CA INDEX NAME)



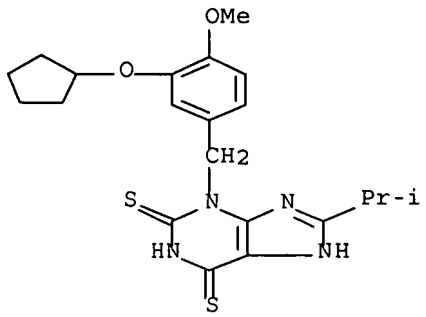
RN 162279-01-8 CAPLUS
CN 1H-Purine-2,6-dithione, 3-butyl-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



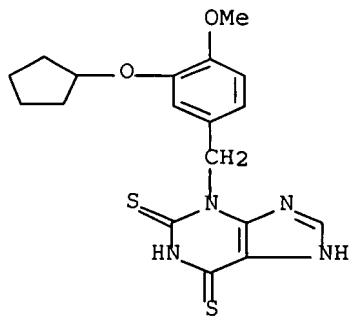
RN 162279-02-9 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



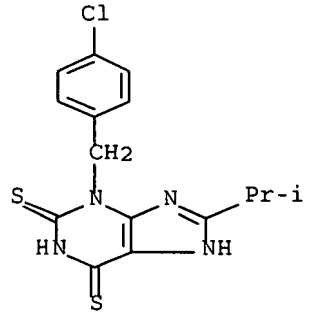
RN 162279-04-1 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



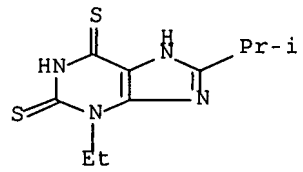
RN 162279-05-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[[3-(cyclopentyloxy)-4-methoxyphenyl]methyl]-3,7-dihydro- (9CI) (CA INDEX NAME)



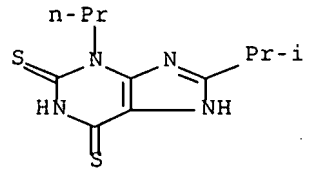
RN 162279-06-3 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[(4-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



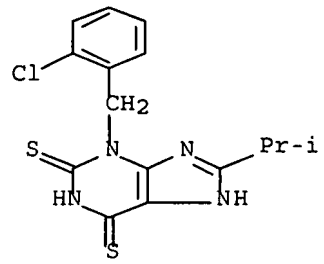
RN 162279-07-4 CAPLUS
CN 1H-Purine-2,6-dithione, 3-ethyl-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



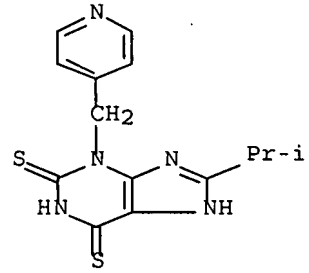
RN 162279-08-5 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-propyl- (9CI) (CA INDEX NAME)



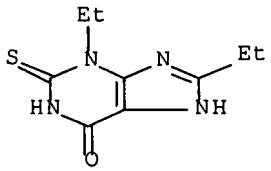
RN 162279-09-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3-[(2-chlorophenyl)methyl]-3,7-dihydro-8-(1-methylethyl)- (9CI) (CA INDEX NAME)



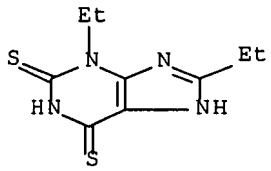
RN 162279-10-9 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-8-(1-methylethyl)-3-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



IT **162278-04-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)
RN 162278-04-8 CAPLUS
CN 6H-Purin-6-one, 3,8-diethyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



IT **162278-92-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of purines, isoguanines, and dithioxanthines as phosphodiesterase-IV inhibitors)
RN 162278-92-4 CAPLUS
CN 1H-Purine-2,6-dithione, 3,8-diethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



L57 ANSWER 25 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:462796 CAPLUS Full-text
DOCUMENT NUMBER: 122:278022
TITLE: Image formation of silver halide photographic materials
INVENTOR(S): Ito, Katsuhiko; Sanpei, Takeshi
PATENT ASSIGNEE(S): Konishiroku Photo Ind, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 27 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06347954	A	19941222	JP 1993-140638	19930611 <--

PRIORITY APPLN. INFO.: JP 1993-140638 19930611 <--
ED Entered STN: 01 Apr 1995
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

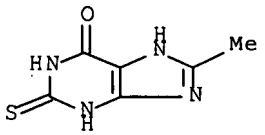
AB The title photog. materials, possessing ≥1 Ag halide emulsion layer on a support and containing a hydrazine derivative ANA1NA2GR [A = aryl, heterocycle containing ≥1 S or O; G = (CO)n, sulfonyl, sulfoxy, P(:O)R1, iminomethylene; n = 1, 2; A1 = A2 = H or when 1 of A1 or A2 is H the other is (substituted) alkylsulfonyl (substituted) acyl; R = H, alkyl, aryl, heterocycle, amino, OR2;

R1 = alkyl, alkenyl, alkynyl, aryl, saturated heterocycle, OR3; R2, R3 = alkyl, alkenyl, alkynyl, aryl, saturated heterocycle], an amine compound R71R72NR73 (R71-73 = H, substituent, R71-73 may form a ring), and an alc. compound R91R92CHOH (R91, R92 = H, substituent) in the emulsion layer and/or other hydrophilic colloid layer, are processed with a developing solution of pH 9.5-12.3 containing dihydroxybnezene-type developing agents, 3-pyrazolidone-type or aminophenol-type developing agents, ≥0.3 mol/L sulfites, and a N-containing heterocyclic compound selected from I, II, and III [R31-34, R41-44, R51-54 = H, SM1, OH, (substituted) alkyl, alkoxy, amino, aryl, SO3M2, CO2M3, ≥1 of R31-34, ≥1 of R41-44, and ≥1 of R51-54 are SM1; M1-3 = H, alkali metal, ammonium]. Even if the materials are processed with developing solns. containing high concns. of sulfites, Ag sludge formation is suppressed and super-high contrast images with high sensitivity are obtained. Thus, a photog. film with a Ag(Cl, I, Br) emulsion layer containing IV and Et2N(CH2)2(OCHMeCH2)7S(CH2)2NEt2 was exposed using a HeNe laser and developed with a developing solution (pH 11.5) containing hydroquinone, 4-methyl-4-hydroxymethyl-1-phenyl-3-pyrazolidone, Na2SO3 (55 g/L), and I (R31 = SH, R32-34 = H).

IT **91184-09-7**
RL: MOA (Modifier or additive use); TEM (Technical or engineered material use); USES (Uses)
(hydroquinone-type photog. developer containing nitrogen-containing heterocyclic compound)

RN 91184-09-7 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 26 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:255796 CAPLUS Full-text
DOCUMENT NUMBER: 122:118847
TITLE: Method of processing silver halide photographic material containing hydrazine with amine-containing developer solution
INVENTOR(S): Kato, Mariko; Ishikawa, Wataru; Sanpei, Takeshi
PATENT ASSIGNEE(S): Konishiroku Photo Ind, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 31 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

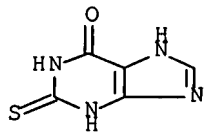
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06250348	A	19940909	JP 1993-36906	19930225 <--

PRIORITY APPLN. INFO.: JP 1993-36906 19930225 <--
ED Entered STN: 21 Dec 1994
AB The claimed method comprises using a developer solution consisting of (1) dihydroxybenzene, (2) derivative of 3-pyrazolidone or aminohenol, (3) ≥0.3

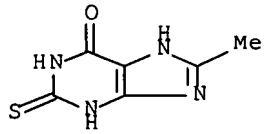
mol/L of sulfite, (4) amine compound R1R2CHANR3R4 and R3R4NANR5R6 (R1 = H, OH, carboxy; R2, R3, R4, R5, R6 = H, monovalent organic group; A = bivalent group; when R3 and R4 are Et, R1 ≠ OH; R3 and R5, and R4 and R6 may be combined to form heterocyclic rings), and (5) a mercapto or thion-substituted N-containing heterocyclic compd having no benzo form condensed ring. The developer solution does not generate silver sludge and reduces black peppers. It has high speed and good stability and provides high contrast images.

IT **2487-40-3 91184-09-7**
RL: MOA (Modifier or additive use); NUU (Other use, unclassified); USES (Uses)
(photog. developer containing amine and sulfur-containing azocyclic compound)

RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 91184-09-7 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-2-thioxo- (9CI) (CA INDEX NAME)



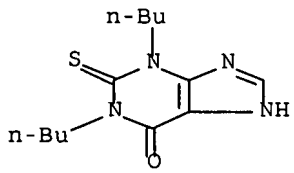
L57 ANSWER 27 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:168945 CAPLUS Full-text
DOCUMENT NUMBER: 122:315012
TITLE: Selective Ligands for Rat A3 Adenosine Receptors: Structure-Activity Relationships of 1,3-Dialkylxanthine 7-Riboside Derivatives
AUTHOR(S): Kim, Hea Ok; Ji, Xiao-duo; Melman, Neli; Olah, Mark E.; Stiles, Gary L.; Jacobson, Kenneth A.
CORPORATE SOURCE: Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD, 20892, USA
SOURCE: Journal of Medicinal Chemistry (**1994**), 37(23), 4020-30
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 08 Nov 1994
AB 1,3-Dialkylxanthine 7-riboside analogs modified at the 1-, 3-, and 8-purine positions and at the ribose 5'-position were synthesized. The nucleoside analogs were examined for affinity in radioligand binding essays at rat brain A3 adenosine receptors stably expressed in CHO cells, using the radioligand

[[125I]-4-amino3-iodobenzyl]adenosine-5'-N-methyluronamide (AB-MECA). The affinity of xanthine 7-ribosides at A3 receptors depended on the 1,3-dialkyl substituents in the order: Pent ≥ Bu » Hx > Pr ≈ Me. 1,3-Dipentylxanthine-7-riboside was slightly selective for A3 receptors (2-fold vs A1 and 10-fold vs A2a). 8-Methoxy substitution was tolerated at A3 receptors. 2-Thio vs 2-oxo substitution increased potency at all three subtypes and slightly increased A3 vs A1 selectivity. The 5'-uronamide modification, which was previously found to enhance A3 selectivity in N6-benzyladenosine derivs., was also incorporated into the xanthine 7-ribosides, with similar results. 1,3-Dibutylxanthine 7-riboside 5'-N-methylcarboxamide, with a Ki value of 229 nM at A3 receptors, was 160-fold selective for rat A3 vs A1 receptors and >400-fold selective vs A2a receptors. This derivative acted as a full agonist in the A3 receptor-mediated activation of adenylate cyclase.

IT **77038-96-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of dialkylxanthine ribosides as selective ligands for A3 adenosine receptors)

RN 77038-96-1 CAPLUS

CN 6H-Purin-6-one, 1,3-dibutyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



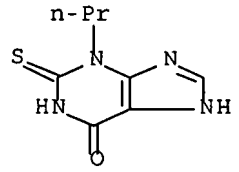
L57 ANSWER 28 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:500054 CAPLUS Full-text
DOCUMENT NUMBER: 121:100054
TITLE: A binding site model and structure-activity relationships for the rat A3 adenosine receptor
AUTHOR(S): van Galen, Philip J. M.; van Bergen, Andrew H.; Gallo-Rodriguez, Carola; Melman, Neli; Olah, Mark E.; Ijzerman, Ad P.; Stiles, Gary L.; Jacobson, Kenneth A.
CORPORATE SOURCE: Lab. Bioorganic Chem., Natl. Inst. Diabetes, Digestive and Kidney Diseases, Bethesda, MD, 20892, USA
SOURCE: Molecular Pharmacology (1994), 45(6), 1101-11
CODEN: MOPMA3; ISSN: 0026-895X
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 03 Sep 1994
AB A novel adenosine receptor, the A3 receptor, has recently been cloned. The authors have systematically investigated the hitherto largely unexplored structure-activity relationships (SARs) for binding at A3 receptors, using 125I-N6-2-(4-aminophenyl)ethyladenosine as a radioligand and membranes from Chinese hamster ovary cells stably transfected with the rat A3-cDNA. As is the case for A1 and A2a receptors, substitutions at the N6 and 5' positions of adenosine, the prototypic agonist ligand, may yield fairly potent compds. However, the highest affinity and A3 selectivity is found for N6,5'-disubstituted compds., in contrast to A2 and A2a receptors. Thus, N6-benzyladenosine-5'-N-ethylcarboxamide is highly potent (Ki, 6.8 nM) and moderately selective (13- and 14-fold vs. A1 and A2a). The N6 region of the

A3 receptor also appears to tolerate hydrophilic substitutions, in sharp contrast to the other subtypes. Potencies of N6,5'-disubstituted compds. in inhibition of adenylate cyclase via A3 receptors parallel their high affinity in the binding assay. None of the typical xanthine or nonxanthine (A1/A2) antagonists tested show any appreciable affinity for rat A3 receptors. 1,3-Dialkylxanthines did not antagonize the A3 agonist-induced inhibition of adenylate cyclase. A His residue in helix 6 that is absent in A3 receptors but present in A1/A2 receptors may be causal in this respect. In a mol. model for the rat A3 receptor, this mutation, together with an increased bulkiness of residues surrounding the ligand, make antagonist binding unfavorable when compared with a previously developed A1 receptor model. Second, this A3 receptor model predicted similarities with A1 and A2 receptors in the binding requirements for the ribose moiety and that xanthine-7-ribosides would bind to rat A3 receptors. This hypothesis was supported exptl. by the moderate affinity (Ki, 6 μM) of 7-riboside of 1,3-dibutylxanthine, which appears to be a partial agonist at rat A3 receptors. The model presented here which is consistent with the detailed SAR found in this study, may serve to suggest future chemical modification, site-directed mutagenesis, and SAR studies to further define essential characteristics of the ligand-receptor interaction and to develop even more potent and selective A3 receptor ligands.

IT **156733-29-8**
RL: BIOL (Biological study)
(adenosine A1 and A2a and A3 receptors affinity for, mol. structure in relation to)

RN 156733-29-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-propyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 29 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:323047 CAPLUS Full-text

DOCUMENT NUMBER: 120:323047

TITLE: Reactions of 6-thiotheophylline with alkylating agents and epichlorohydrin: isolation of S-alkylated 6-thiotheophylline and 7-(2,3-thioepoxypropyl)theophylline

AUTHOR(S): Hayashi, Hiroaki; Suzuki, Fumio; Yasuzawa, Toru; Ueno, Hideo

CORPORATE SOURCE: Pharm. Res. Lab., Kyowa Hakko Kogyo Co., Ltd., Nagaizumi, 411, Japan

SOURCE: Journal of Heterocyclic Chemistry (1993), 30(1), 247-51
CODEN: JHTCAD; ISSN: 0022-152X

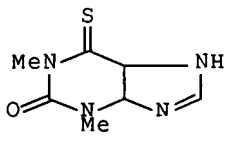
DOCUMENT TYPE: Journal

LANGUAGE: English

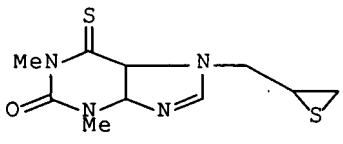
OTHER SOURCE(S): CASREACT 120:323047

ED Entered STN: 25 Jun 1994

GI



I



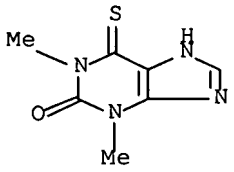
II

AB Alkylation of 6-thiotheophylline (I) under the aprotic basic condition affords S-alkyl-6-thiotheophylline together with an N7-alkylated product. There is a tendency that the more reactive the alkylating agents are, the higher the yields of S-alkylated products are. However, treatment of I with epichlorohydrin afforded an unexpected product, 7-(2,3-thioepoxypropyl)theophylline (II), neither an S-alkylated compound nor an N7-alkylated compound The chemical structure was determined by NMR spectroscopic anal.

IT **2398-70-1**, 6-Thiotheophylline
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of thiotheophylline with alkylating agents and epichlorohydrin)

RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 30 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:127807 CAPLUS Full-text

DOCUMENT NUMBER: 120:127807

TITLE: Herbicidal δ-aminolevulinic acid combinations with chlorophyll biosynthesis modulators.

INVENTOR(S): Rebeiz, Constantin A.

PATENT ASSIGNEE(S): Board of Trustees of the University of Illinois, USA

SOURCE: U.S., 40 pp. Cont.-in-part of U.S. 5,163,990.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5242892	A	19930907	US 1990-615413	19901119 <--
EP 331211	A2	19890906	EP 1989-106579	19850717 <--
EP 331211	A3	19891123		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
ZA 8505561	A	19860326	ZA 1985-5561	19850723 <--
US 5127938	A	19920707	US 1986-895529	19860811 <--

US 5200427	A	19930406	US 1989-294132	19890109 <--
US 5163990	A	19921117	US 1990-521119	19900503 <--
CA 2080140	A1	19911104	CA 1991-2080140	19910502 <--
CA 2080140	C	20020108		
WO 9116820	A1	19911114	WO 1991-US3015	19910502 <--
W: CA, JP, KR				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
EP 527186	A1	19930217	EP 1991-909022	19910502 <--
R: BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL				
JP 06500989	T	19940127	JP 1991-508902	19910502 <--
CA 2358003	C	20020924	CA 1991-2358003	19910502 <--
US 5286708	A	19940215	US 1991-773030	19911008 <--
US 5300526	A	19940405	US 1991-795367	19911120 <--
US 5321001	A	19940614	US 1992-915896	19920717 <--
JP 2001151614	A	20010605	JP 2000-226123	20000621 <--
JP 3365503	B2	20030114		
JP 2003063907	A	20030305	JP 2002-236923	20020815 <--
JP 3734780	B2	20060111		

PRIORITY APPLN. INFO.:	US 1984-634932	B2	19840727 <--
	US 1985-754092	B1	19850715 <--
	US 1986-895529	A2	19860811 <--
	US 1990-521119	A2	19900503 <--
	EP 1985-903637	P	19850717 <--
	US 1988-144883	B2	19880113 <--
	US 1989-294132	A3	19890109 <--
	US 1990-615413	A	19901119 <--
	CA 1991-2080140	A3	19910502 <--
	JP 1991-508902	A3	19910502 <--
	WO 1991-US3015	W	19910502 <--
	JP 2000-226123	A3	20000621 <--

ED Entered STN: 19 Mar 1994

AB The title compns. are defoliants and herbicides, with activity based on the accumulation of photodynamic tetrapyrrols. A mixture of 20 mM γ-aminolevulinic acid and 15 mM 6-aminonicotinic acid defoliated tomato seedlings.

IT **152968-88-2**

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(herbicide and defoliant)

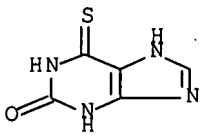
RN 152968-88-2 CAPLUS

CN Pentanoic acid, 5-amino-4-oxo-, mixt. with 1,3,6,7-tetrahydro-6-thioxo-2H-purin-2-one (9CI) (CA INDEX NAME)

CM 1

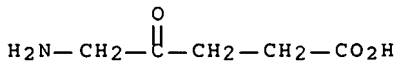
CRN 2002-59-7

CMF C5 H4 N4 O S

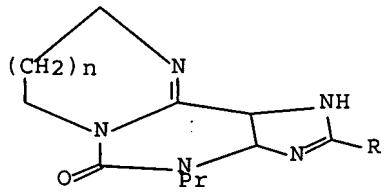


CM 2

CRN 106-60-5
CMF C5 H9 N O3



L57 ANSWER 31 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:77080 CAPLUS Full-text
DOCUMENT NUMBER: 120:77080
TITLE: Convenient synthesis of tricyclic purine derivatives
AUTHOR(S): Shimada, Junichi; Kuroda, Takeshi; Suzuki, Fumio
CORPORATE SOURCE: Pharm. Res. Lab., Kyowa Hakko Kogyo Co., Ltd., Shizuoka, 411, Japan
SOURCE: Journal of Heterocyclic Chemistry (1993), 30(1), 241-6
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:77080
ED Entered STN: 19 Feb 1994
GI



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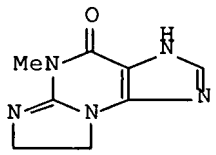
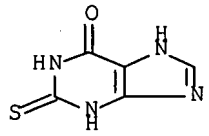


II

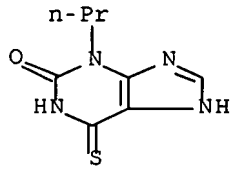
AB A convenient synthesis of the title compds. I (R = H, cyclopentyl; n = 0-2) and II is described. The syntheses of I and II were accomplished by treatment of 6-methylthio-7H-purin-2(3H)-ones or 2-benzylthio-1-methyl-9-triphenylmethyl-9H-purin-6(1H)-one (III) with the appropriate amino alc. followed by dehydrative cyclization using SOCl2. III was efficiently prepared by benzylation of 6-hydroxy-2-mercaptopurine followed by tritylation and N-methylation.

IT **2487-40-3**, 6-Hydroxy-2-mercaptopurine
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylation of)

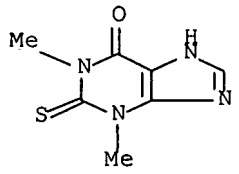
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



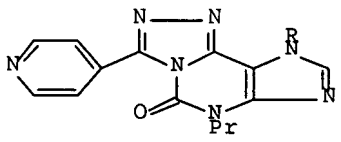
IT **105396-65-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation of)
RN 105396-65-4 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 32 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:644995 CAPLUS Full-text
DOCUMENT NUMBER: 117:244995
TITLE: Approach to an adenosine pharmacophore by molecular modeling
AUTHOR(S): Neuwels, M.
CORPORATE SOURCE: UCB Sect. Pharm., Chemin Foriest, Braine-l-Alleud, B-1420, Belg.
SOURCE: Journal de Pharmacie de Belgique (**1992**), 47(4), 351-63
CODEN: JPBEAJ; ISSN: 0047-2166
DOCUMENT TYPE: Journal
LANGUAGE: French
ED Entered STN: 26 Dec 1992
AB The selective development of adenosine A1 antagonists was carried out in 2 steps. First an A1 pharmacophore common to various known chemical families was determined in order to permit the design of new chemical skeletons; then a predictive modeling of affinities was carried out to select new potential ligands. The mol. modeling was done on 6 different chemical families (triazoloquinoxalines, adenines, xanthines, pyrazolopyrimidinones, triazoloquinazolines, and imidazoquinolines), and a search for a common superimposition was carried out. Starting from the different superpositions obtained, a CoMFA study (QSAR-3D) allowed the building of predictive models for A1 receptor affinity. The theor. preferred superposition proved to be the best, as it was able to correctly predict the activities of new ligands.
IT **6603-63-0**
RL: BIOL (Biological study)
(in mol. modeling of adenosine receptor pharmacophore)
RN 6603-63-0 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 33 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:469819 CAPLUS Full-text
DOCUMENT NUMBER: 117:69819
TITLE: Facile synthesis of 9H-s-triazolo[3,4-i]purin-5(6H)-ones
AUTHOR(S): Shimada, Junichi; Suzuki, Fumio
CORPORATE SOURCE: Pharm. Res. Lab., Kyowa Hakko Kogyo Co., Ltd., Shizuoka, 411, Japan
SOURCE: Tetrahedron Letters (1992), 33(22), 3151-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:69819
ED Entered STN: 23 Aug 1992
GI



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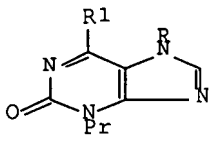
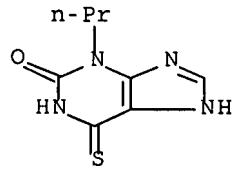


II

AB New tricyclic heterocycles, 9H-s-triazolo[3,4-i]purin-5(6H)-ones I (R = Me, H), were prepared from 6-methylthio-7H-purin-2(3H)-ones II (R = Me, PhCH2OCH2; R1 = MeS) via cyclization of II (R1 = isonicotinoylhydrazino).
IT **105396-65-4**, 3-Propyl-6-thioxanthine
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation or benzylation of)
RN 105396-65-4 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 34 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:426495 CAPLUS Full-text

DOCUMENT NUMBER: 117:26495
TITLE: Facile and general synthesis of 8-substituted 2-(methylthio)purin-6-ones
AUTHOR(S): Nagamatsu, Tomohisa; Yamasaki, Hiroo
CORPORATE SOURCE: Fac. Pharm. Sci., Okayama Univ., Tsushima, 700, Japan
SOURCE: Heterocycles (1992), 33(2), 775-90
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:26495
ED Entered STN: 26 Jul 1992
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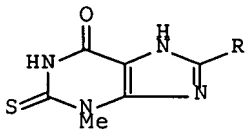

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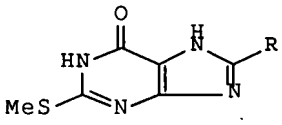
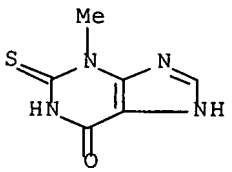


II

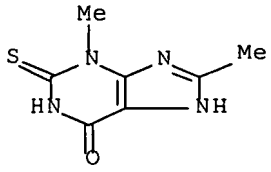
AB 3-Methyl-6-oxo-2-thioxo-1,2,3,6-tetrahydropurines [I; R = H, alkyl, (un)substituted Ph] were synthesized by oxidative cyclization of 5,6-diamino-1-methyl-2-thiouracil-RCHO reaction products or 6-amino-5-(benzylideneamino)-1-methyl-2-thiouracils in the presence of di-Et azodicarboxylate (DEAD). In addition, the oxidative cyclization of 4-amino-5-(benzylideneamino)-3-methyl-2-(methylthio)pyrimidin-6(3H)-ones in the presence of DEAD gave 8-aryl-3-methyl-2-(methylthio)-6-oxo-3,6- dihydropurines, which were identical with the compds. prepared by methylation of I. 2-(Methylthio)-6-oxo-1,6-dihydropurines [II; R = H, alkyl, (un)substituted Ph] were synthesized from 4,5-diamino-2-(methylthio)pyrimidin-6(1H)-one or 4-amino-5-(benzylideneamino)-2-(methylthio)pyrimidin-6(1H)-ones in a similar manner as above.

IT **28139-02-8P 91725-06-3P 103289-69-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)

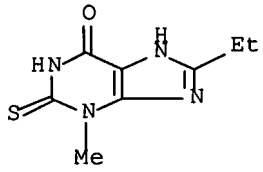
RN 28139-02-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



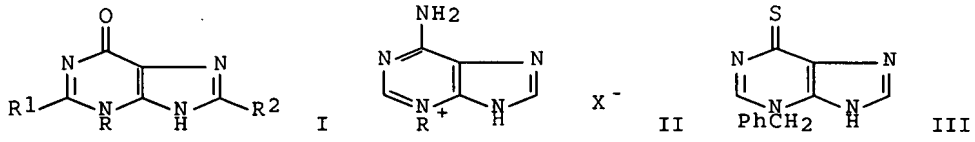
RN 91725-06-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3,8-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 103289-69-6 CAPLUS
CN 6H-Purin-6-one, 8-ethyl-1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 35 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:214213 CAPLUS Full-text
DOCUMENT NUMBER: 116:214213
TITLE: Inhibitors of human purine nucleoside phosphorylase. Synthesis and biological activities of 8-amino-3-benzylhypoxanthine and related analogs
AUTHOR(S): Woo, Peter W. K.; Kostlan, Catherine R.; Sircar, Jagadish C.; Dong, Mi K.; Gilbertsen, Richard B.
CORPORATE SOURCE: Parke-Davis Pharm. Res. Div., Warner-Lambert Co., Ann Arbor, MI, 48105, USA
SOURCE: Journal of Medicinal Chemistry (1992), 35(8), 1451-7
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:214213
ED Entered STN: 31 May 1992
GI

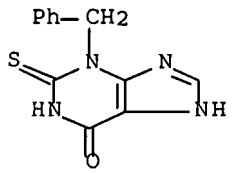


AB 3-Substituted hypoxanthines I (R = CH2Ph, CH2C6H3Cl2-3,4, CH2C6H4CN-4, CH2C6H4NO2-4, CH2C6H4OMe-4, CH2CH2Ph, 2-thienylmethyl, 2-furylmethyl; R1 = H, SMe, OH, NH2; R2 = H, NH2, NHCHO) and analogs II (R = CH2Ph, X = Cl; R = CH2C6H4NO2-4, X = Br) and III have been synthesized as inhibitors of purine nucleoside phosphorylase (PNP), which may conceivably act as T-cell-selective immunosuppressive agents with potential utility in autoimmune disorders such

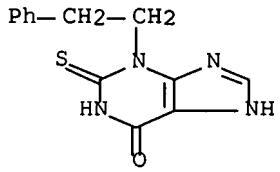
as rheumatoid arthritis, in organ transplantations, and in T-cell leukemias. The compds. were evaluated for their PNP activity by a radiochem. assay and also for their cytotoxic effects on a T-lymphoblastoid cell line (MOLT-4). Appropriate substitutions on 3-benzylhypoxanthine (I, R = CH2Ph, R1, R2 = H) increase potency. Variation of the 3-aryl substituents of I (R = CH2Ph, R1, R2 = H) failed to further increase potency. Replacement of the 6-oxygen function in I (R = CH2Ph, R1,R2 = H) to give II or III resulted in little change in activity. Other variations resulted in decreased activity. I (R = CH2Ph, 2-thienylmethyl, 2-furylmethyl, CH2C6H4OMe-4, R1, R2 = NH2) have moderate but significant activities, as compared to the most active inhibitor presently known, 8-amino-9-thienylguanine. I (R1, R2 = NH2) represent a novel structural type which were prepared via formation of the aminoimidazole moiety through a base-catalyzed 1,5-(O → N)-carbamimidoyl rearrangement.

IT **28741-76-6P 139460-82-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, reductive dethiolation, and purine nucleoside phosphorylase-inhibiting activity of)

RN 28741-76-6 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(phenylmethyl)-2-thioxo- (9CI) (CA INDEX NAME)



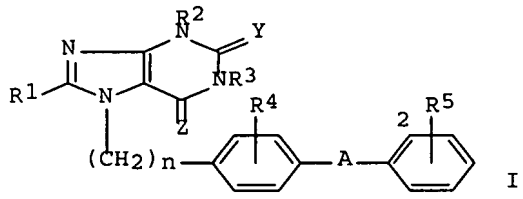
RN 139460-82-5 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(2-phenylethyl)-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 36 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:582959 CAPLUS Full-text
DOCUMENT NUMBER: 115:182959
TITLE: Preparation of xanthine derivatives as angiotensin II antagonists
INVENTOR(S): Morimoto, Akira; Nishikawa, Kohei
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: Eur. Pat. Appl., 38 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 430300	A2	19910605	EP 1990-123013	19901130 <--
EP 430300	A3	19920325		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 03223284	A	19911002	JP 1990-338861	19901130 <--
CA 2031328	A1	19910602	CA 1990-2031328	19901203 <--
PRIORITY APPLN. INFO.:			JP 1989-313918 A	19891201 <--

OTHER SOURCE(S): MARPAT 115:182959
ED Entered STN: 01 Nov 1991
GI

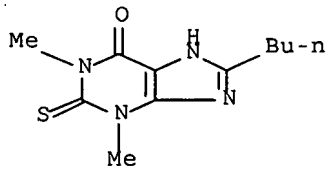


I

AB Xanthine derivs. [I; R1 = (substituted) hydrocarbyl, optionally bound through a hetero atom; one of R2 and R3 = (substituted) hydrocarbyl, the other is H or (substituted) hydrocarbyl; R4 = H, halo, NO2; R5 = a group capable of forming an anion; A = bond, a spacer having atomic length ≤2; n = 1, 2; Y, Z = O, S], useful in treating hypertension, heart diseases, strokes, etc., are prepared To a solution of cyano compound I (R1 = Bu, R2 = R3 = Me, R4 = H, R5 = 2-cyano, A = bond, Y = Z = O, n = 1) in DMF were added NaN3 and NH4Cl with stirring at 115° to give 59.8% tetrazole derivative I [R1 = Bu, R2 = R3 = Me, R4 = H, R5 = 2-(1H-tetraol-5-yl), A = bond, Y = Z = O, n = 1], which showed IC50 of 2.8 + 10-7 M against angiotensin II binding. Capsule, tablet, and injection formulations were given.

IT **136420-18-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of angiotensin II antagonist)

RN 136420-18-3 CAPLUS
CN 6H-Purin-6-one, 8-butyl-1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)

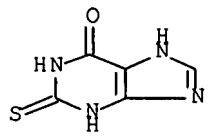


L57 ANSWER 37 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:536115 CAPLUS Full-text
DOCUMENT NUMBER: 115:136115
TITLE: Preparation of condensed purine derivatives as drugs
INVENTOR(S): Suzuki, Fumio; Shimada, Junichi; Kuroda, Takeshi;

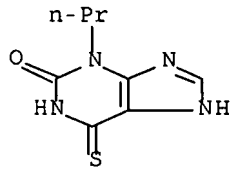
Kubo, Kazuhiro; Karasawa, Akira; Ohno, Tetsuji; Ohmori, Kenji
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 43 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 423805	A2	19910424	EP 1990-120056	19901019 <--
EP 423805	A3	19920102		
EP 423805	B1	20000823		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
CA 2028235	A1	19910421	CA 1990-2028235	19901019 <--
CA 2028235	C	19970121		
JP 03204880	A	19910906	JP 1990-281578	19901019 <--
US 5270316	A	19931214	US 1990-599758	19901019 <--
AT 195739	T	20000915	AT 1990-120056	19901019 <--
ES 2152207	T3	20010201	ES 1990-120056	19901019 <--

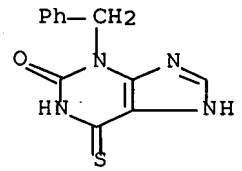
PRIORITY APPLN. INFO.: JP 1989-273403 A 19891020 <--
OTHER SOURCE(S): MARPAT 115:136115
ED Entered STN: 05 Oct 1991
GI For diagram(s), see printed CA Issue.
AB Title compds. I (A = Q, Q1, Q2; R1 = H, alkyl, alicyclic alkyl, noradamantan-3-yl, dicyclopropylmethyl, styryl; R2 = H, alkyl, alicyclic alkyl; R3 = H, alkyl, PhCH2; X1, X2 = H, alkyl, aralkyl, Ph; n = 0, 1) or a salt thereof, useful as diuretics, renal protecting agents, bronchodilators or hypotensives, are prepared Thus, H2NCH2CH2OH was added to 3,7-dihydro-7-methyl-6-(methylthio)-3-propyl-2H-purin-2-one (preparation given) and treated at 160° for 1 h to give the hydroxyethylamino derivative which was refluxed with POCl3 and after workup to give the imidazaopurinone II. II showed biol. activity as the above agents. Pharmaceutical formulations are given.
IT **2487-40-3**, 2-Mercapto-6-hydroxypurine
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylation of)
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



IT **105396-65-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation of)
RN 105396-65-4 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



IT **19844-94-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of condensed purines as drugs)
RN 19844-94-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(phenylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)

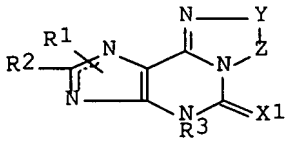


L57 ANSWER 38 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:491963 CAPLUS Full-text
DOCUMENT NUMBER: 115:91963
TITLE: Preparation and formulation of s-triazolo[3,4-i]purine derivatives as bronchodilators, diuretics, renal protectants, and antiamnestic agents
INVENTOR(S): Suzuki, Fumio; Shimada, Junichi; Ohmori, Kenji; Manabe, Haruhiko; Kubo, Kazuhiro; Karasawa, Akira; Ohno, Tetsuji; Shiozaki, Shizuo; Ishii, Akio; Shuto, Katsuichi
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 52 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

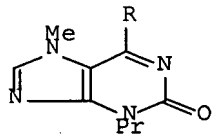
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 417790	A2	19910320	EP 1990-117662	19900913 <--
EP 417790	A3	19920318		
EP 417790	B1	19961204		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 03204879	A	19910906	JP 1990-243248	19900913 <--
JP 2980658	B2	19991122		
AT 145908	T	19961215	AT 1990-117662	19900913 <--
ES 2097124	T3	19970401	ES 1990-117662	19900913 <--
CA 2025413	A1	19910315	CA 1990-2025413	19900914 <--
CA 2025413	C	19971104		
US 5173492	A	19921222	US 1991-752180	19910823 <--

PRIORITY APPLN. INFO.: JP 1989-239117 A 19890914 <--
JP 1989-261761 A 19891006 <--
US 1990-581562 B1 19900912 <--

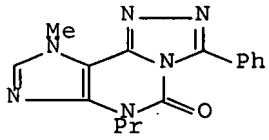
OTHER SOURCE(S): MARPAT 115:91963
ED Entered STN: 06 Sep 1991
GI



I



II



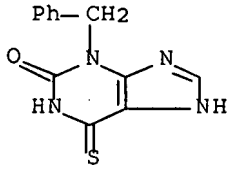
III

AB The title compds. [I; R1, R2 = H, alkyl, cycloalkyl, aralkyl, (substituted) aryl; R3 = alkyl, cycloalkyl, aralkyl, (substituted) aryl; X1 = O, S; YZ = N:CR4 or NR4C(:X2) wherein R4 = H, alkyl, (substituted) (hetero)aryl, X2 = O, S, NH] are prepared PhCONHNH2 was added to a suspension of II (R = MeS) (preparation given) in MePh, the mixture was refluxed to give 60% hydrazine derivative II (R = PhCONHNH), which (2.64 g) was refluxed with 308 mg p-MeC6H4SO3H in MePh to give 67% title compound III. III showed IC50 of 4.1 μM in passive Schultz-Dale reaction (bronchodilatory effects) and diuretic activity at 25 mg/kg orally in rats. Also prepared and tested were 50 addnl. I. Tablet, syrup, powder, and capsule formulations were also given.

IT **19844-94-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of triazolopurine drugs)

RN 19844-94-1 CAPLUS

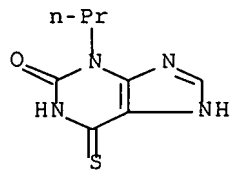
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(phenylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



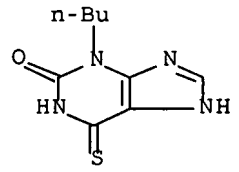
IT **105396-65-4 135445-55-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of triazolopurine drugs)

RN 105396-65-4 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)

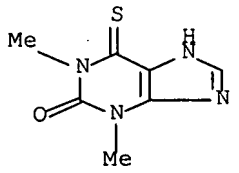


RN 135445-55-5 CAPLUS
CN 2H-Purin-2-one, 3-butyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)

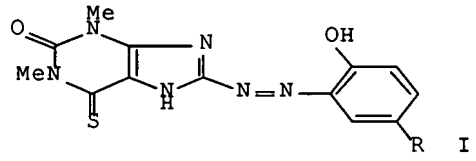


L57 ANSWER 39 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:111839 CAPLUS Full-text
DOCUMENT NUMBER: 112:111839
TITLE: Pharmacological effects and binding studies of new methylxanthine thioderivatives
AUTHOR(S): Ragazzi, E.; Froldi, G.; Santi Soncin, E.; Borea, P. A.; Fassina, G.
CORPORATE SOURCE: Dep. Pharmacol., Univ. Padua, Padua, I-35131, Italy
SOURCE: Pharmacological Research (1989), 21(6), 707-17
CODEN: PHMREP; ISSN: 1043-6618
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 31 Mar 1990
AB The pharmacol. effects of 2 methylxanthine derivs., 6-thiocaffeine (TC) and 6-thiotheophylline (TT), were studied in different in vitro and in vivo conditions. On guinea-pig isolated trachea, both TC and TT showed a relaxant effect (EC50 50 μM and 60 μM, resp.), more potent than theophylline (300 μM). In guinea-pig isolated atria, TC (30-50 μM) antagonized N6-phenylisopropyladenosine (a stable agonist on adenosine receptors) neg. effect in not a clearly competitive way. Higher concentration (100 μM) began to reverse that inhibitory effect. In vitro Ki of TC and TT for A1 and A2 adenosine receptors was intermediate in comparison to caffeine and theophylline. On the contrary, the 2 thioderivs. showed a higher affinity for [3H]-nitrendipine binding sites, in comparison to the original methylxanthines; this can be responsible for an antagonism at the level of Ca2+ L-type channels, at concns. <1 mM, when caffeine and theophylline are not effective. In vivo expts. in mice provided evidence for a lack of CNS stimulant effects, but a loss of motor coordination was observed Both thioderivs. showed a reduced acute toxicity.
IT **2398-70-1**, 6-Thiotheophylline
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pharmacol. of, mechanisms in)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)

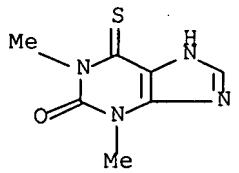


L57 ANSWER 40 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:55760 CAPLUS Full-text
DOCUMENT NUMBER: 112:55760
TITLE: Synthesis of new thiotheophylline azo compounds and their application as photometric reagents for vanadium(V)
AUTHOR(S): Guseinov, I. K.; Agaragimov, M. A.; Askerov, D. N.
CORPORATE SOURCE: Inst. Neorg. Fiz. Khim., Baku, USSR
SOURCE: Azerbaidzhanskii Khimicheskii Zhurnal (1988), (1), 131-7
CODEN: AZKZAU; ISSN: 0005-2531
DOCUMENT TYPE: Journal
LANGUAGE: Russian
ED Entered STN: 17 Feb 1990
GI



I

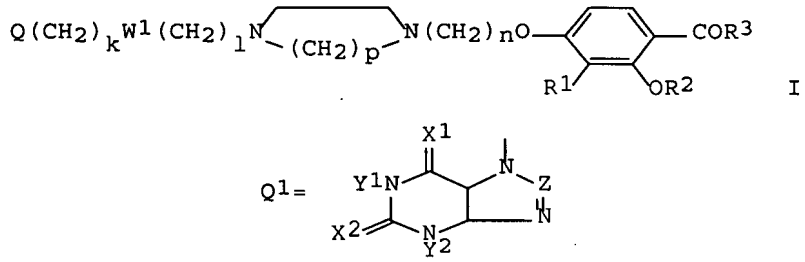
AB The title compds. I (R = H, Cl, SO3H, NO2) were prepared in 32-48% yields by coupling reactions of 6-thiotheophylline, prepared in 91% yield by sulfuration of theophylline with P2S5, with diazotized aminophenols. I are useful in photometric determination of vanadium(V).
IT **2398-70-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and coupling reaction with diazotized aminophenols)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 41 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:35563 CAPLUS Full-text
DOCUMENT NUMBER: 112:35563
TITLE: Preparation of xanthine derivatives as leukotriene antagonists
INVENTOR(S): Suzuki, Fumio; Shimada, Junichi; Hayashi, Hiroaki; Oomori, Takemori; Manabe, Haruhiko
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01156978	A	19890620	JP 1988-169572	19880707 <--
PRIORITY APPLN. INFO.:			JP 1987-239270	A1 19870924 <--

OTHER SOURCE(S): MARPAT 112:35563
ED Entered STN: 04 Feb 1990
GI

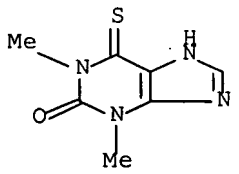


I

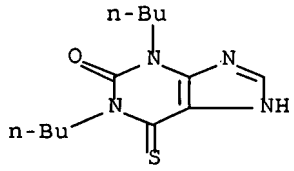
AB The title compds. I [Q = xanthine, 8-azaxanthine residue (e.g., Q1, etc.); Z = N, CY3; Y1-Y3 = H, alkyl, alkenyl, etc.; X1, X2 = O, S; W1, W2, CH2, CHOA, etc.; A = H, acyl; R1 = alkyl, alkenyl; R2 = H, acyl; R3 = H, alkyl, cycloalkyl; k, l, m, n = 0-4; p = 1-3] and salts thereof, useful as leukotriene antagonists, were prepared A mixture of 1,3-dimethyl-7-(3-iodopropyl)xanthine, 2-hydroxy-3-propyl-4-[3-(1-piperazinyl)propoxy]acetophenone, and Et3N in EtOH was refluxed for 2.5 h to give, after acidification with HCl, 69% 7-[3-[4-[3-(4-acetyl-3-hydroxy- 2-propylphenoxy)propyl]1-piperazinyl]propyl]-1,3-dimethylxanthine-3HCl (II). II exhibited an IC50 of 0.93 μM against leukotriene D4 in a test using guinea pig tracheal strips.

IT **2398-70-1 40915-18-2**

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of leukotriene antagonist)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)

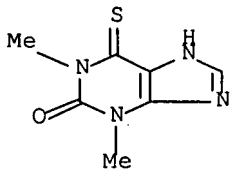


RN 40915-18-2 CAPLUS
CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 42 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:542347 CAPLUS Full-text
DOCUMENT NUMBER: 109:142347
TITLE: New methylxanthine thio-derivatives inducing marked tracheal relaxation without increasing cardiac inotropism or motor activity
AUTHOR(S): Ragazzi, E.; Froldi, G.; Soncin, E. Santi; Fassina, G.
CORPORATE SOURCE: Dep. Pharmacol., Univ. Padua, Padua, Italy
SOURCE: Pharmacological Research Communications (1988), 20(7), 621-2
CODEN: PLRCAT; ISSN: 0031-6989
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 28 Oct 1988
AB The methylxanthine derivative 6-thiocaffine at 0.01-1 mM had neg. inotropic and chronotropic effects on isolated guinea pig atria, whereas 6-thiotheopylline had neg. effects only at high concns. (>1 mM). In addition, 6-thiocaffeine at 3-100 μM increased the heart rate, did not affect contraction, and reduced perfusion pressure in isolated guinea pig hearts. Both methylxanthines relaxed the guinea pig trachea with EC50 of .apprx.50 μM. The LD50 values for 6-thiocaffeine and 6-thiotheophylline were 365 and 430 mg/kg, i.p., resp. Neither compound increased locomotor activity, and 6-thiotheophylline caused a behavioral depression.
IT **2398-70-1**, 6-Thiotheophylline
RL: PRP (Properties)
(trachea relaxation from and cardiac effects of)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX

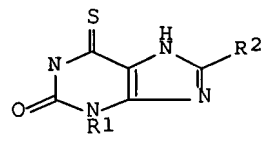
NAME)



L57 ANSWER 43 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:406542 CAPLUS Full-text
DOCUMENT NUMBER: 109:6542
TITLE: Preparation, formulation, and testing of 6-thioxanthine bronchodilators
INVENTOR(S): Hofer, Peter
PATENT ASSIGNEE(S): Euro-Celtique S. A., Luxembourg
SOURCE: Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
EP 256692	A2	19880224	EP 1987-306557		19870724	<--
EP 256692	A3	19890830				
EP 256692	B1	19920916				
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE						
DK 8703677	A	19880203	DK 1987-3677		19870715	<--
DK 161965	B	19910902				
DK 161965	C	19920210				
ZA 8705346	A	19880330	ZA 1987-5346		19870721	<--
CA 1276147	C	19901113	CA 1987-542734		19870722	<--
AT 80632	T	19921015	AT 1987-306557		19870724	<--
ES 2046204	T3	19940201	ES 1987-306557		19870724	<--
US 4925847	A	19900515	US 1987-78545		19870728	<--
AU 8776286	A	19880204	AU 1987-76286		19870730	<--
AU 601456	B2	19900913				
JP 63041478	A	19880222	JP 1987-191515		19870730	<--
JP 2590120	B2	19970312				
US 5010081	A	19910423	US 1989-415970		19891002	<--
PRIORITY APPLN. INFO.:			GB 1986-18931	A	19860802	<--
			US 1985-699254	A2	19850207	<--
			EP 1987-306557	A	19870724	<--
			US 1987-78545	A1	19870728	<--
			US 1989-322364	B2	19890313	<--

OTHER SOURCE(S): MARPAT 109:6542
ED Entered STN: 09 Jul 1988
GI



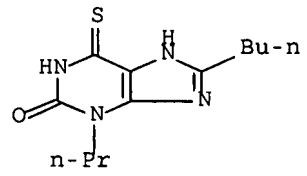
I

AB The title compds. (I; R1 = C2-6 alkyl, C3-7 cycloalkyl, C4-8 cycloalkylalkyl; R2 = C1-6 alkyl, C3-7 cycloalkyl, C4-8 cycloalkylalkyl; provided that when R1 = Et, Pr, or Bu, R2 = C3-6 alkyl, C3-7 cycloalkyl, or C4-8 cycloalkylalkyl) were prepared as bronchodilators. 3-Ethyl-8-butylxanthine and P2S5 were refluxed in pyridine to give 70% 3-ethyl-8-butyl-6-thioxanthine. The latter was 55.0 times as active in relaxing isolated guinea pig tracheal tissue than theophylline.

IT **114834-11-6P 114834-12-7P 114834-13-8P**
114834-14-9P 114834-17-2P 114834-18-3P
114834-19-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as bronchodilator)

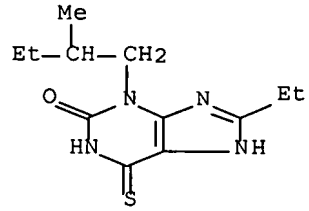
RN 114834-11-6 CAPLUS

CN 2H-Purin-2-one, 8-butyl-1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



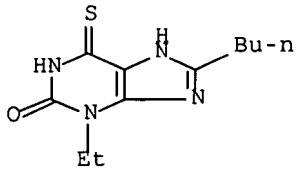
RN 114834-12-7 CAPLUS

CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-3-(2-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)

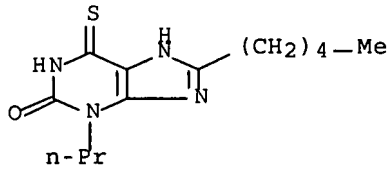


RN 114834-13-8 CAPLUS

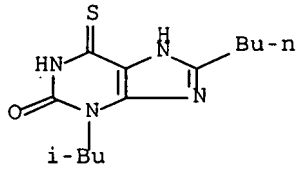
CN 2H-Purin-2-one, 8-butyl-3-ethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



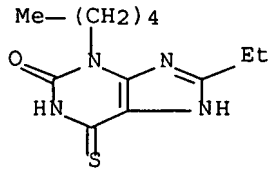
RN 114834-14-9 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-8-pentyl-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



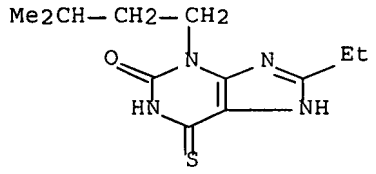
RN 114834-17-2 CAPLUS
CN 2H-Purin-2-one, 8-butyl-1,3,6,7-tetrahydro-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



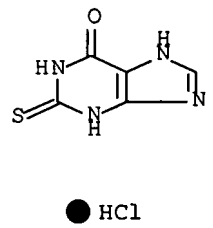
RN 114834-18-3 CAPLUS
CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-3-pentyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 114834-19-4 CAPLUS
CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-3-(3-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)

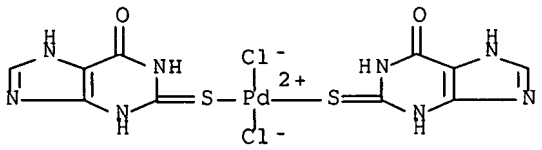


L57 ANSWER 44 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:86769 CAPLUS Full-text
DOCUMENT NUMBER: 108:86769
TITLE: The 2-thioxanthine and its chlorohydrate. Synthesis, characterization and complexing behavior with palladium(II), rhodium(III), gold(III) and platinum(IV)
AUTHOR(S): Sanchez Sanchez, M. P.; Salas Peregrin, J. M.; Romero Molina, M. A.
CORPORATE SOURCE: Fac. Cienc., Univ. Granada, Spain
SOURCE: Anales de Quimica, Serie B: Quimica Inorganica y Quimica Analitica (1987), 83(2), 129-34
CODEN: AQSAD3; ISSN: 0211-1349
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
ED Entered STN: 05 Mar 1988
AB 2-Thioxanthine hydrochloride (TXH2Cl), Pd(TXH)2Cl2.2H2O, Rh(TX)2Cl.3H2O, Au(TX)Cl2, and Pt(TX)2Cl2.H2O were prepared These compds. and TXH were characterized by elemental anal. and spectral (electronic, NMR, IR) methods. The thermal decomposition of the complexes was also studied.
IT **104187-16-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectra of)
RN 104187-16-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo-, monohydrochloride (9CI) (CA INDEX NAME)

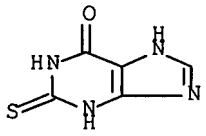


● HCl

IT **112614-64-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and thermolysis and spectra of)
RN 112614-64-9 CAPLUS
CN Palladium, dichlorobis(1,2,3,7-tetrahydro-2-thioxo-6H-purin-6-one-S)-, (SP-4-1)- (9CI) (CA INDEX NAME)



IT **2487-40-3**, 2-Thioxanthine
RL: PRP (Properties)
(reaction with hydrochloric acid and spectra of)
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)

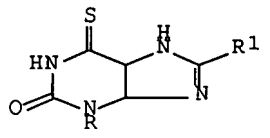


L57 ANSWER 45 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:626214 CAPLUS Full-text
DOCUMENT NUMBER: 105:226214
TITLE: 6-Thioxanthine derivatives
INVENTOR(S): Hofer, Peter
PATENT ASSIGNEE(S): Euro-Celtique S. A., Luxembourg
SOURCE: Eur. Pat. Appl., 7 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 191313	A1	19860820	EP 1986-100544	19860117 <--
EP 191313	B1	19921028		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4710503	A	19871201	US 1985-699254	19850207 <--
IN 161914	A1	19880227	IN 1985-CA906	19851218 <--
ZA 8509805	A	19860827	ZA 1985-9805	19851223 <--
IL 77430	A	19881031	IL 1985-77430	19851224 <--
AU 8651840	A	19860814	AU 1986-51840	19860103 <--
AU 570142	B2	19880303		
AT 81858	T	19921115	AT 1986-100544	19860117 <--
FI 8600285	A	19860808	FI 1986-285	19860121 <--
FI 84180	B	19910715		
FI 84180	C	19911025		
DK 8600332	A	19860808	DK 1986-332	19860122 <--
DK 161964	B	19910902		
DK 161964	C	19920210		
CN 86101050	A	19861112	CN 1986-101050	19860205 <--
CN 1013676	B	19910828		
NO 8600424	A	19860808	NO 1986-424	19860206 <--
NO 163569	B	19900312		

NO 163569	C	19900620			
CA 1275288	C	19901016	CA 1986-501288		19860206 <--
JP 61183287	A	19860815	JP 1986-24248		19860207 <--
JP 07080882	B	19950830			
US 4820709	A	19890411	US 1987-75937		19870722 <--
US 4925847	A	19900515	US 1987-78545		19870728 <--
US 5010081	A	19910423	US 1989-415970		19891002 <--
JP 08099882	A	19960416	JP 1995-6756		19950119 <--
JP 2888273	B2	19990510			
PRIORITY APPLN. INFO.:			US 1985-699254	A	19850207 <--
			EP 1986-100544	A	19860117 <--
			GB 1986-18931	A	19860802 <--
			US 1987-78545	A1	19870728 <--
			US 1989-322364	B2	19890313 <--

OTHER SOURCE(S): CASREACT 105:226214
ED Entered STN: 26 Dec 1986
GI

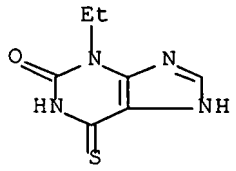


I

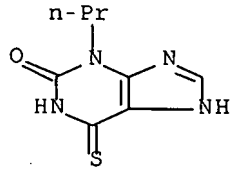
AB The title compds. I (R = Et, Pr, Bu; R1 = H, Me, Et) useful as bronchodilators (no data) were prepared Thus, 3-ethylxanthine in pyridine was treated with P2S5, H2O, NaOH, and acidified with 5N HCl to give I (R = Et; R1 = H).

IT **105396-64-3P 105396-65-4P 105396-66-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as bronchodilator)

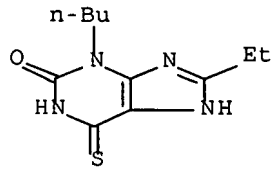
RN 105396-64-3 CAPLUS
CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



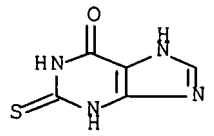
RN 105396-65-4 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



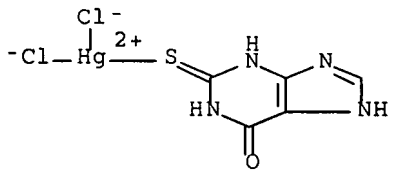
RN 105396-66-5 CAPLUS
CN 2H-Purin-2-one, 3-butyl-8-ethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



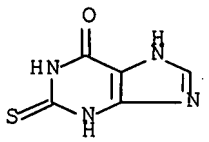
L57 ANSWER 46 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:563883 CAPLUS Full-text
DOCUMENT NUMBER: 105:163883
TITLE: Thermal studies on purine complexes. XI. Thermal behavior of 2-thioxanthine, its chlorohydrate and some thioxanthine complexes of silver(I), cadmium(II), mercury(II) and mercury(I)
AUTHOR(S): Sanchez-Sanchez, M. P.; Salas-Peregrin, J. M.; Romero-Molina, M. A.
CORPORATE SOURCE: Fac. Sci., Univ. Granada, Granada, 18071, Spain
SOURCE: Thermochimica Acta (1986), 102, 149-62
CODEN: THACAS; ISSN: 0040-6031
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 01 Nov 1986
AB The hydrochloride of 6-oxo-2-thiopurine (LH) was prepared in an acid medium, as well as some Ag(I), Cd(II), Hg(II), and Hg(I) complexes of LH. These compds. were characterized by IR and 1H NMR spectroscopic techniques and thermal anal. (thermogravimetry (TG), differential TG, DSC). Dehalogenation enthalpies were calculated
IT **2487-40-3DP**, mercury and silver complexes **104626-28-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition of)
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 104626-28-0 CAPLUS
CN Mercury, dichloro(1,2,3,7-tetrahydro-2-thioxo-6H-purin-6-one-S)- (9CI) (CA INDEX NAME)

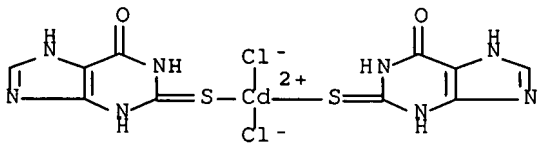


IT **104187-16-8P 104626-27-9P 104626-29-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, heat of dechlorination and thermal decomposition of)
RN 104187-16-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo-, monohydrochloride (9CI) (CA INDEX NAME)

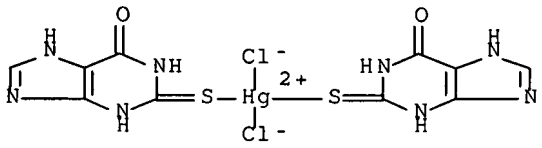


● HCl

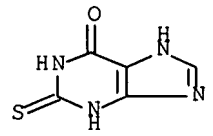
RN 104626-27-9 CAPLUS
CN Cadmium, dichlorobis(1,2,3,7-tetrahydro-2-thioxo-6H-purin-6-one-S)-, (T-4)- (9CI) (CA INDEX NAME)



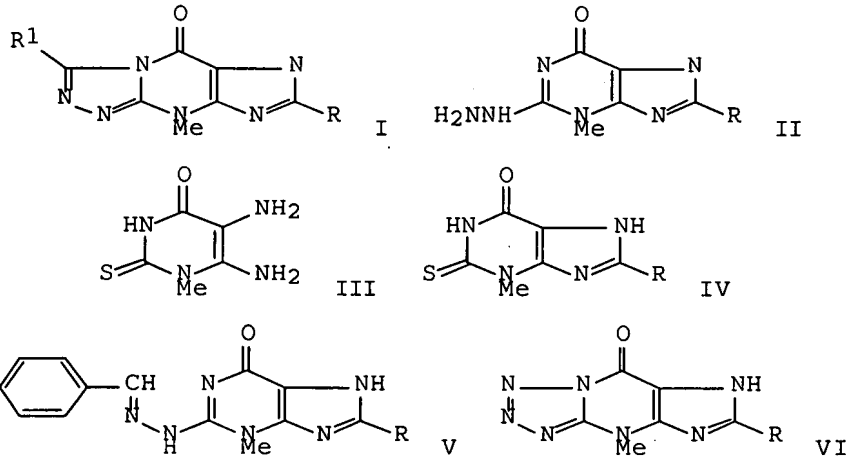
RN 104626-29-1 CAPLUS
CN Mercury, dichlorobis(1,2,3,7-tetrahydro-2-thioxo-6H-purin-6-one-S)-, (T-4)- (9CI) (CA INDEX NAME)



IT 2487-40-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with hydrochloric acid, heat of fusion and thermal study of)
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 47 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:478896 CAPLUS Full-text
DOCUMENT NUMBER: 105:78896
TITLE: Syntheses of 4-methyl-s-triazolo[4,3-a]purin-9(4H)-ones and tetrazolo[1,5-a]purin-9(4H)-ones as aza analogs of "Y" bases
AUTHOR(S): Nagamatsu, Tomohisa; Ukai, Masayoshi; Yoneda, Fumio; Brown, Desmond J.
CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(8), 3113-21
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:78896
ED Entered STN: 06 Sep 1986
GI

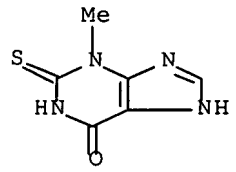


AB 4-Methyl-s-triazolo[4,3-a]purin-9(4H)-ones I (R = H, Me, Et, Ph; R1 = H, Me, Et) were prepared by the cyclocondensation of purin-6(3H)-ones II (R = same) with the appropriate R1C(OEt)3. II were prepared by cyclizing pyrimidine III with RC(OEt)3 and treating the resulting thioxanthines IV with NH2NH2. I [R =

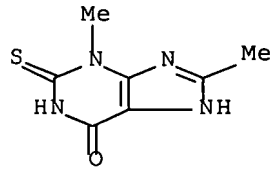
Me, Et, Ph; R1 = p-R2C6H4 (R2 = H, Me, Cl, OMe)] were prepared by the condensation of the appropriate II with p-R2C6H4CHO, followed by the oxidative cyclization of the resulting arylidenehydrazine derivs. V. I (R = Me, Et; R1 = SH, SMe, SEt, SCH2CONH2) were also prepared Tetrazolo[1,5-a]purin-9(4H)-ones VI (R = H, Me, Et, Ph) were prepared by treating the corresponding II with NaNO2/HCl.

IT **28139-02-8P 91725-06-3P 103289-69-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with hydrazine)

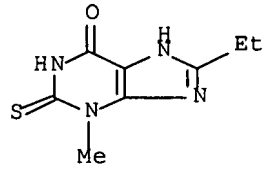
RN 28139-02-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 91725-06-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3,8-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)

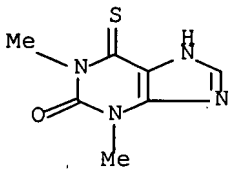


RN 103289-69-6 CAPLUS
CN 6H-Purin-6-one, 8-ethyl-1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)

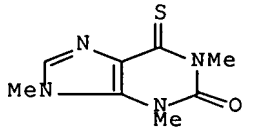


L57 ANSWER 48 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:178050 CAPLUS Full-text
DOCUMENT NUMBER: 104:178050
TITLE: 1,3-Dimethyl-2-oxo-6-thioxo-1,2,3,6-tetrahydropurine (S-theophylline)
AUTHOR(S): Benetollo, F.; Bombieri, G.; Dell'Acqua, L.; Fassina,

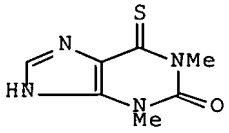
G.
CORPORATE SOURCE: Inst. Chem. Technol. Radioelec., CNR, Padua, 35100, Italy
SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (1986), C42(3), 325-7
CODEN: ACSCEE; ISSN: 0108-2701
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 17 May 1986
AB The title compound is orthorhombic, space group Pbn21, with a 15.614(3), b 8.338(2), and c 6.570(2) Å; dc = 1.52 for Z = 4. Final R = 0.053 for 650 reflections. Atomic coordinates are given. The bond lengths and angles are normal for purine derivs., with the 5- and 6-membered rings and S atom planar. The S-theophylline mols., in contrast to the theophylline ones, are linked in chains by intermol. H bonding (N...O 2.704(9) Å), but do not form the dimers found in the theophylline structure.
IT **2398-70-1**
RL: PRP (Properties)
(crystal structure of)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 49 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:571723 CAPLUS Full-text
DOCUMENT NUMBER: 103:171723
TITLE: A caffeine analog (1,3,7-trimethyl-6-thioxo-2-oxopurine) with a negative inotropic and chronotropic effect
AUTHOR(S): Fassina, G.; Gaion, R. M.; Caparrotta, L.; Carpenedo, F.
CORPORATE SOURCE: Dep. Pharmacol., Univ. Padova, Padua, I-35131, Italy
SOURCE: Naunyn-Schmiedeberg's Archives of Pharmacology (1985), 330(3), 222-6
CODEN: NSAPCC; ISSN: 0028-1298
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 30 Nov 1985
GI



I



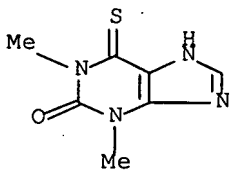
II

AB Cardiac effects of thioxanthine derivs., 6-thiocaffeine (I) [13182-58-6] and 6-thiotheophylline (II) [2398-70-1], were studied on isolated guinea pig atria and on partially purified cardiac cAMP phosphodiesterase [9036-21-9] enzymes. Theophylline [58-55-9] and caffeine [58-08-2] were used as reference compds. On elec. driven left atria I (0.01-1 mmol/L) decreased contractile tension in a concentration dependent manner. On spontaneously beating atria, the same concns. of I showed neg. inotropic as well as neg. chronotropic effects. On elec. driven left atria, II (0.01-1 mmol/L) increased heart contractile tension but, at higher concns., a reversal of the stimulating effect was observed Both I and II inhibited bovine heart cAMP phosphodiesterase activity to a comparable extent. Their inhibitory potencies were about 2 and 9-fold higher than those of theophylline or caffeine but consistently lower than that of IBMX. Thus, the replacement of O and S in the methylxanthine mol. drastically modifies the effect induced by the drugs on cardiac function without changing those on cAMP phosphodiesterase.

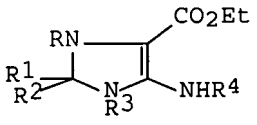
IT **2398-70-1**
RL: BIOL (Biological study)
(heart rate and contraction response to)

RN 2398-70-1 CAPLUS

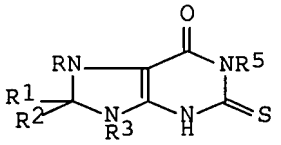
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



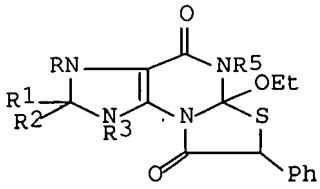
L57 ANSWER 50 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:630460 CAPLUS Full-text
DOCUMENT NUMBER: 101:230460
TITLE: Studies on ring-fused mesoionic thiazolo[3,2-a]imidazolo[4,5-d]pyrimidine derivatives
AUTHOR(S): Talukdar, P. B.; Sengupta, S. K.; Datta, A. K.
CORPORATE SOURCE: Res. Dev. Div., East India Pharm. Works Ltd., Calcutta, 700 061, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1984), 23B(4), 316-20
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:230460
ED Entered STN: 22 Dec 1984
GI



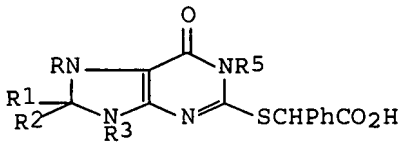
I



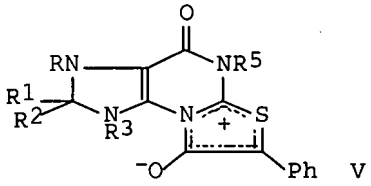
II



III



IV



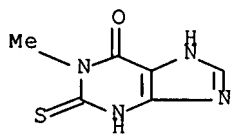
V

AB Aminoimidazole esters I (RR1, R1R3 = bond; R = Me; R2 = H, CH2Ph, SMe; R3 = H, Me; R4 = H) were treated with isothiocyanates R5NCS (R5 = Me, Ph) to give thiourea derivs. I [R4 = C(S)NHR5], which cyclized to give oxopurines II. The oxopurines underwent cyclocondensation with ClCHPhCO2Et to give imidazopyrimidine lactams III, which were hydrolyzed to give thiopurines IV. Cyclodehydration of IV (RR1 = bond; R2 = R3 = H; R5 = Me, Ph) gave the N-acylated mesoionic compds. V (R = Ac; R1R3 = bond; R2 = H; R5 = Me, Ph), and thiopurines IV (RR1 = bond, R2 = PhCH2, R3 = H, R5 = Me; R = Me, R1R3 = bond, R2 = CH2Ph, R5 = Me) gave the non-acylated V (R = H) on similar treatment. Treating the mesoionic compds. with EtOH regenerated the imidazopyrimidine lactams.

IT **91184-08-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with chloro(phenyl)acetate, imidazopyrimidine lactam by)

RN 91184-08-6 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-2-thioxo- (9CI) (CA INDEX NAME)



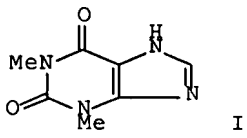
L57 ANSWER 51 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1983:154921 CAPLUS Full-text

DOCUMENT NUMBER: 98:154921

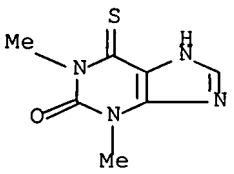
TITLE: New derivatives of methylxanthines: effect of thiocaffeine, thiotheophylline, and 8-phenyltheophylline on lipolysis and on phosphodiesterase activities

AUTHOR(S): Scotini, E.; Carpenedo, F.; Fassina, G.
CORPORATE SOURCE: Inst. Pharmacol., Padua Univ., Padua, Italy
SOURCE: Pharmacological Research Communications (1983), 15(2), 131-43
CODEN: PLRCAT; ISSN: 0031-6989
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI



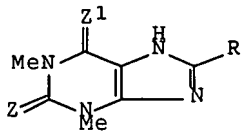
I

AB The effects of theophylline (I)(TH) [58-55-9], caffeine (CAFF) [58-08-2], 6-thiotheophylline (S-TH) [2398-70-1], 6-thiocaffeine (S-CAFF) [13182-58-6], 8-phenyltheophylline (8-PT) [961-45-5], 3-isobutyl-1-methylxanthine (IBMX) [28822-58-4] on spontaneous and norepinephrine [51-41-2]-induced lipolysis and on cAMP phosphodiesterase (cAMP-PDE) [9036-21-9] activities of rat fat cells were studied. These agents stimulated lipolysis. 8-PT was the most potent compound Thiocaffeine and thiotheophylline had the least potent activities. IBMX and theophylline had intermediate potencies. The order of potency of the same drugs in potentiating norepinephrine-stimulated lipolysis was: IBMX > 8-PT > S-CAFF > > S-TH > CAFF > TH. The rank order of potency to inhibit cAMP-PDE was: IBMX > S-TH and S-CAFF > TH » 8-PT (ineffective). Thus, thiocaffeine and thiotheophylline were more potent than the parent compound theophylline in inhibiting cAMP-PDE, although lipolysis stimulating activities of these compds. were much lower. In contrast, 8-PT stimulated both spontaneous and norepinephrine-induced lipolysis, even though the compound did not inhibit PDE. Some correlation was observed between the order of the antiadenosine activity of these compds. as reported in the literature and their ability to stimulate basal lipolysis. Both antiadenosine and antiPDE activities appear to be involved in modulating hormone-induced lipolysis.
IT **2398-70-1**
RL: BIOL (Biological study)
(lipolysis by and PDE activities in adipose tissue response to)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 52 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1983:125211 CAPLUS Full-text

DOCUMENT NUMBER: 98:125211
TITLE: Comparison of the mass spectra of 6-thiotheophyllines and 6-sulfinyltheophyllines
AUTHOR(S): Bergmann, Felix; Rahat, Miriam; Frank, Arie; Deutsch, Joseph
CORPORATE SOURCE: Dep. Pharmacol., Hebrew Univ.-Hadassah Med. Sch., Jerusalem, Israel
SOURCE: Organic Mass Spectrometry (**1982**), 17(11), 565-8
CODEN: ORMSBG; ISSN: 0030-493X
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI

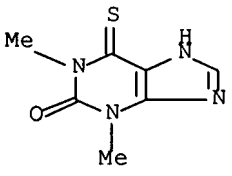


I

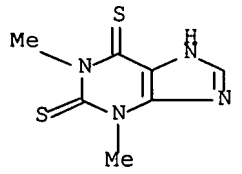
AB Under electron impact, 6-thiotheophyllines (I; Z = O, S; Z1 = S; R = H, Ph) eliminate various fragments from the pyrimidine moiety. In a retro-Diels-Alder reaction, they lose the fragment Z:C:NMe3 from positions 1 and 2 of the pyrimidine ring. In 6-sulfinyltheophyllines (I; Z = O, S; Z1 = SO; R = H, Ph) the sulfinyl group is the main target for fragmentation; it loses either O or S, and the abundance of [M-16]+ and [M-32]+ is much higher than that of the mol. ion. Elimination of the S of the 6-sulfinyl substituent, with retention of its O, is due to formation of a cyclic C-O-S intermediate. All further fragmentations of I (Z1 = SO) proceed via primary O or S loss, followed by elimination of fragments from the pyrimidine moiety, similar to the primary processes observed in the mass spectra of I (Z1 = S).

IT **2398-70-1 6501-94-6 14156-64-0**
84959-31-9
RL: PRP (Properties)
(mass spectrum of, fragmentation mechanism in)

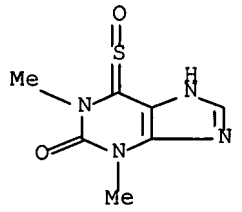
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



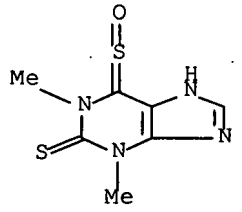
RN 6501-94-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



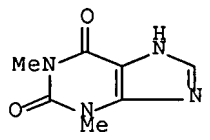
RN 14156-64-0 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-sulfinyl- (9CI) (CA INDEX NAME)



RN 84959-31-9 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl-, S6-oxide (9CI) (CA INDEX NAME)



L57 ANSWER 53 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1983:119142 CAPLUS Full-text
DOCUMENT NUMBER: 98:119142
TITLE: Alkylxanthines as adenosine receptor antagonists and membrane phosphodiesterase inhibitors in central nervous tissue: evaluation of structure-activity relationships
AUTHOR(S): Wu, P. H.; Phillis, J. W.; Nye, M. J.
CORPORATE SOURCE: Coll. Med., Univ. Saskatchewan, Saskatoon, SK, Can.
SOURCE: Life Sciences (1982), 31(25), 2857-67
CODEN: LIFSAK; ISSN: 0024-3205
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI

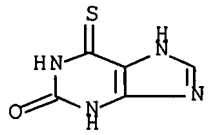


I

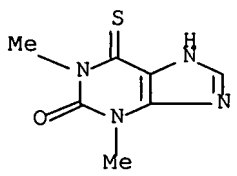
AB A series of alkylxanthines were examined as antagonists of the adenosine [58-61-7] A1-receptor in rat brain synaptosomal membranes and as inhibitors of membrane phosphodiesterase [9025-82-5]. Structure-activity relations showed that the addition of certain substituting groups at position 8 of the theophylline mol. produced mol. structures which generally favored adenosine receptor antagonism. This is evident from the potency order of 8-substituted theophyllines as adenosine receptor antagonists: 8-(p-bromophenyl)theophylline [63325-99-5], 8-(p- methylphenyl)theophylline [57196-70-0], 8-phenyltheophylline [961-45-5] and 8-(p-chlorophenyltheophylline [29064-02-6], 8- (methoxyphenyl)theophylline [84942-90-5] > 8-(dimethylaminophenyl)theophylline [54013-59-1] > 8-benzyltheophylline [2879-15-4] > theophylline (I) [58-55-9]. The order of potency for inhibition of brain membrane phosphodiesterase was: 1,3-dimethyl-2,6- dithioxopurine [**6501-94-6**] > methylxanthines > 8-substituted theophyllines. 8-Substituted theophyllines may be selective in their activity as adenosine receptor antagonists, whereas an increase in lipid solubility by substitution at the 1, 2, 3, and 6 positions of the purine ring may result in an increase in phosphodiesterase inhibition.

IT **2002-59-7 2398-70-1 2487-40-3**
5437-25-2 6501-94-6 6603-63-0
RL: BIOL (Biological study)
(adenosine receptor and phosphodiesterase of synaptosome membrane response to, alkylxanthines effect on)

RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)

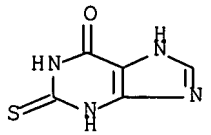


RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)

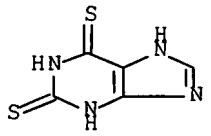


RN 2487-40-3 CAPLUS

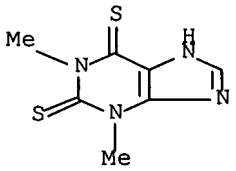
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



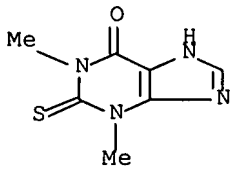
RN 5437-25-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



RN 6501-94-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 6603-63-0 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



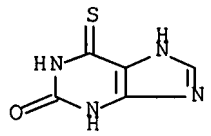
L57 ANSWER 54 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:435269 CAPLUS Full-text
DOCUMENT NUMBER: 95:35269
TITLE: Adenosine antagonism by purines, pteridines, and benzopteridines in human fibroblasts
AUTHOR(S): Bruns, Robert F.
CORPORATE SOURCE: Dep. Neurosci., Univ. California, La Jolla, CA, 92093,

USA
SOURCE: Biochemical Pharmacology (1981), 30(4), 325-33
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984

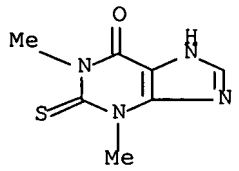
AB Testing of >100 purine bases and structurally related heterocycles as adenosine (I) [58-61-7] antagonists in VA13 fibroblasts (determined by cAMP increase) yielded 3 families of I antagonists: xanthines, benzo[g]pteridines, and 9-substituted adenines. For the xanthines, the optimal group at the 1-position was Bu (5-fold improvement vs. Me), at the 7-position was 2-chloroethyl (5-fold improvement vs. H), and at the 8-position was p-bromophenyl (100-fold improvement vs. H). The receptors apparently had butyl- and phenyl-sized pockets at the 1- and 8-positions, resp., since compds. with larger groups had greatly reduced activity.

IT **2002-59-7 6603-63-0 42458-91-3**
RL: BIOL (Biological study)
(adenosine receptor of fibroblast antagonism by)

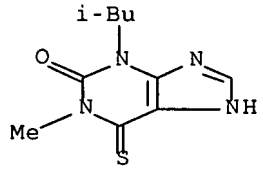
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



RN 6603-63-0 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



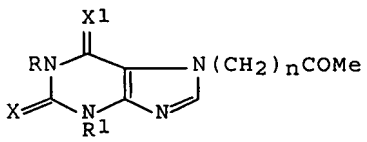
RN 42458-91-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 55 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:139844 CAPLUS Full-text
DOCUMENT NUMBER: 94:139844
TITLE: Xanthine derivatives and their use in pharmaceutical compositions
INVENTOR(S): Goring, Joachim Ewald
PATENT ASSIGNEE(S): Wuelfing, Johann A., Fed. Rep. Ger.
SOURCE: Eur. Pat. Appl., 30 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 18136	A1	19801029	EP 1980-301053	19800402 <--
EP 18136	B1	19831116		
R: AT, BE, CH, DE, FR, GB, IT, NL, SE				
CA 1128509	A1	19820727	CA 1980-348928	19800401 <--
DK 8001485	A	19801006	DK 1980-1485	19800402 <--
DK 147795	B	19841210		
DK 147795	C	19850819		
ES 490290	A1	19811016	ES 1980-490290	19800402 <--
AU 8057190	A	19810115	AU 1980-57190	19800403 <--
AU 531481	B2	19830825		
ZA 8002010	A	19810429	ZA 1980-2010	19800403 <--
JP 55141487	A	19801105	JP 1980-45090	19800405 <--
US 4454138	A	19840612	US 1982-363125	19820429 <--
PRIORITY APPLN. INFO.:			GB 1979-12052 A	19790405 <--
			GB 1979-19505 A	19790605 <--
			US 1980-135285 A1	19800331 <--

OTHER SOURCE(S): MARPAT 94:139844
ED Entered STN: 12 May 1984
GI

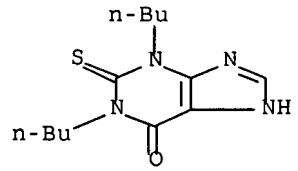


I

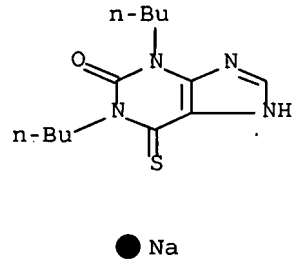
AB Thioxanthine I (X, X1 = O, S; n = 1, 2; R, R1 = alkyl) were prepared Thus, 4 g 1-butyl-3-ethyl-6-thioxanthine was treated with 2.7 g BrCH2COMe to give 1 g I (R = Bu, R1 = Et, X = O, X1 = S, n = 2; II). At 2 mg/kg orally II caused a 22.2% increase in the contractility of skeletal muscle in cats.

IT **77038-96-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with bromopropanone)

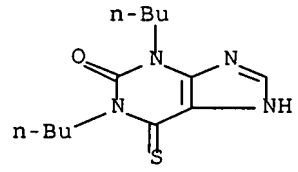
RN 77038-96-1 CAPLUS
CN 6H-Purin-6-one, 1,3-dibutyl-1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



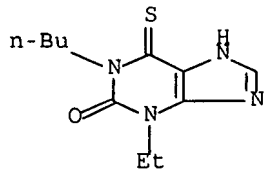
IT **77038-98-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with chloropropanone)
RN 77038-98-3 CAPLUS
CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo-, sodium salt (9CI) (CA INDEX NAME)



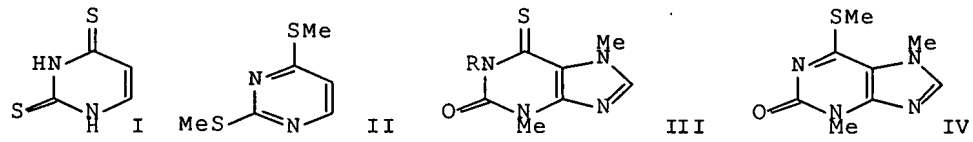
IT **40915-18-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Me vinyl ketone)
RN 40915-18-2 CAPLUS
CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



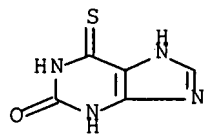
IT **77038-90-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bromopropanone)
RN 77038-90-5 CAPLUS
CN 2H-Purin-2-one, 1-butyl-3-ethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



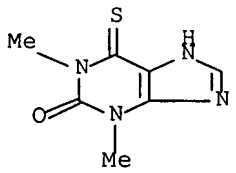
L57 ANSWER 56 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:84065 CAPLUS Full-text
DOCUMENT NUMBER: 94:84065
TITLE: Methylation of thiouracils and thioxanthines with trimethyl phosphate
AUTHOR(S): Hayashi, Masahiro; Hisanaga, Yorisato; Yamauchi, Kiyoshi; Kinoshita, Masayoshi
CORPORATE SOURCE: Dep. Appl. Chem., Osaka City Univ., Osaka, 558, Japan
SOURCE: Synthetic Communications (1980), 10(10), 791-8
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI



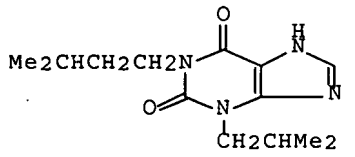
AB Thiouracils and thioxanthines were methylated with (MeO)3PO in DMF at 80-100° to give S-methylated derivs. Thus, I gave 85% II. III (R = H) in the presence of Et3N gave 51% III (R = Me) and 35% IV.
IT **2002-59-7 2398-70-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation of)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 57 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:51769 CAPLUS Full-text
DOCUMENT NUMBER: 92:51769
TITLE: Effects of phosphodiesterase inhibitors on cyclic nucleotide levels and relaxation of pig coronary arteries
AUTHOR(S): Kramer, G. L.; Wells, J. N.
CORPORATE SOURCE: Sch. Med., Vanderbilt Univ., Nashville, TN, 37232, USA
SOURCE: Molecular Pharmacology (1979), 16(3), 813-22
CODEN: MOPMA3; ISSN: 0026-895X
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI

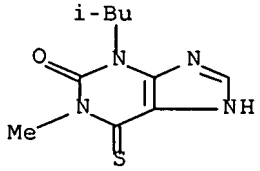


I

AB A series of xanthine derivs. and papaverine were studied to determine their abilities to alter tissue levels of cyclic AMP [60-92-4] and cyclic GMP [7665-99-8], inhibit cyclic nucleotide phosphodiesterase [50812-31-2] activities, and cause relaxation of pig coronary arteries. The agents exhibited a wide range of potencies to inhibit phosphodiesterase activities in the coronary artery supernatant fraction. In addition, some of these agents were up to 10 times more potent as inhibitors of cyclic GMP hydrolysis than of cyclic AMP hydrolysis, whereas others were 2-4 times more potent as inhibitors of cyclic AMP than of cyclic GMP hydrolysis. The rank order of potencies of these agents to cause relaxation of coronary artery strips was similar to the rank order of potencies to inhibit cyclic nucleotide phosphodiesterase activities. There were, however, some notable exceptions to the correlation between inhibition of cyclic nucleotide phosphodiesterase activities and relaxation. 1-Isoamyl-3-isobutylxanthine (I) [63908-26-9] was a more potent relaxing agent than might be expected from its relatively low potency to inhibit cyclic nucleotide hydrolysis in tissue exts. On the other hand, 1-methyl-3-isobutyl-7-(3-chlorobenzyl)-xanthine [58481-28-0] was 1 of the more potent inhibitors of cyclic nucleotide hydrolysis but was not as potent in causing relaxation as might have been expected. Exposure of the coronary artery strips to inhibitors caused increase in tissue levels of cyclic AMP and cyclic GMP and there was a statistically significant multiple linear regression of cyclic AMP and cyclic GMP levels on percent relaxation after 5

min of exposure to the agents. Cyclic AMP and cyclic GMP levels made approx. equal contributions to the regression of changes in percent relaxation, as determined by anal. of variance methods. While I did not fit the correlation between phosphodiesterase inhibition and potency to relax the arterial strips as well as the other agents, this agent caused unexpectedly large increases in cyclic AMP levels. Some agents caused relaxation accompanied by significant elevation of cyclic GMP levels and no significant change in cyclic AMP levels while other agents caused relaxation accompanied by significant increases in cyclic AMP but not cyclic GMP. These data offer some support for a hypothesis that both cyclic AMP and cyclic GMP are involved in the relaxation processes of pig coronary arteries.

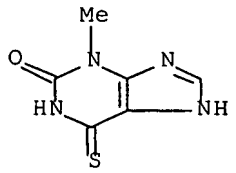
IT **42458-91-3**
RL: BIOL (Biological study)
(cyclic nucleotide of artery and artery contraction response to)
RN 42458-91-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



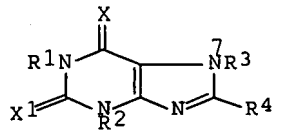
L57 ANSWER 58 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1979:570643 CAPLUS Full-text
DOCUMENT NUMBER: 91:170643
TITLE: Behavior of N-methylated allopurinols and related 4-thioxopyrazolo[3,4-d]pyrimidines towards bovine milk xanthine oxidase
AUTHOR(S): Bergmann, Felix; Frank, Arie; Govrin, Hanna
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Biochimica et Biophysica Acta, Enzymology (1979), 570(1), 215-20
CODEN: BBEZAD; ISSN: 0924-1086
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
AB All available N-mono- and N,N'-dimethylallopurinols and the corresponding 4-thioxo derivs. were tested as substrates or inhibitors of bovine milk xanthine oxidase (EC 1.2.3.2). None of the compds. tested revealed any inhibitory activity towards the enzyme. All compds. were resistant to enzymic oxidation, with the exception of 7-methylallopurinol and its 4-thioxo analog. Both these compds. were attacked at position 6. 7-Methylallopurinol was oxidized nearly 10-fold faster than the isomeric 3-methylhypoxanthine. These observations can be explained by assuming that for attack at C-6, the enzyme must bind both to N-1 and N-2 in the pyrazole ring and causes tautomerization, which places a double bond at position 5,6 in the pyrimidine ring. This activation process resembles the activation of hypoxanthine.

IT **33285-76-6**
RL: BIOL (Biological study)
(xanthine oxidase response to)
RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX

NAME)



L57 ANSWER 59 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:453218 CAPLUS Full-text
DOCUMENT NUMBER: 87:53218
TITLE: 6-Sulfinyl derivatives of xanthines
AUTHOR(S): Bergmann, Felix; Frank, Arie; Weiler-Feilchenfeld, Hanna; Tamir, Ilana
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Journal of Organic Chemistry (1977), 42(14), 2470-3
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI

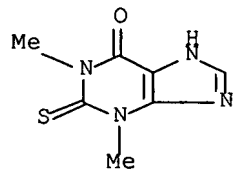


I, X=S
II, X=SO

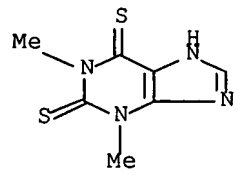
AB 6-Thiopurines I (R1 = R4 = H, R2 = R3 = Me, X1 = O; R1 = R2 = Me, R3 = R4 = H, X1 = O, S; R1 = R2 = Me, R3 = H, R4 = Ph, X1 = O, S) are oxidized by H2O2 or by BzOOH to 6-sulfinylpurines II. Only theophylline derivs. of these unstable II were obtained in pure form. The isomers formed have the 6-sulfinyl group directed toward the 7-NH due to stabilization by an intramol. H bridge. Their structure has been derived from dipole moments and from the chemical shift of the 1-Me substituent. The 2-thiocarbonyl group in 2-thiotheophyllines is not attacked by the oxidants used, which convert 6-selenoxanthines to the corresponding xanthines.

IT **6603-63-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)

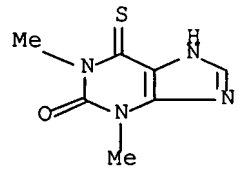
RN 6603-63-0 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



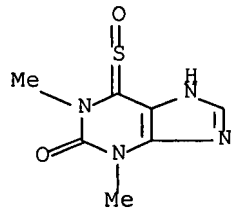
IT **6501-94-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
RN 6501-94-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



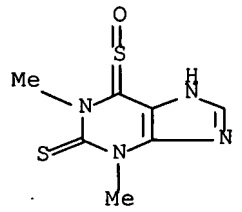
IT **2398-70-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



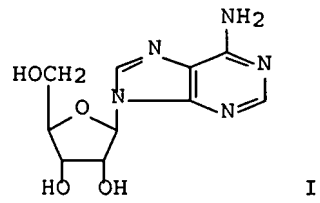
IT **62006-25-1P 62006-26-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 62006-25-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-sulfinyl-, (E)- (9CI) (CA INDEX NAME)



RN 62006-26-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl-, S6-oxide, (E)- (9CI) (CA INDEX NAME)



L57 ANSWER 60 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:133356 CAPLUS Full-text
DOCUMENT NUMBER: 86:133356
TITLE: Effects of adenosine and related compounds on adenylate cyclase and cyclic AMP levels in smooth muscle
AUTHOR(S): McKenzie, Sheila G.; Frew, Robert; Bar, Hans P.
CORPORATE SOURCE: Dep. Pharmacol., Univ. Alberta, Edmonton, AB, Can.
SOURCE: European Journal of Pharmacology (1977), 41(2), 193-203
CODEN: EJPHAZ; ISSN: 0014-2999
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI



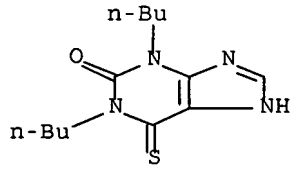
I

AB The hypotheses were tested that the relaxant effect of adenosine (I) [58-61-7] and related compds. in the longitudinal muscle of the rabbit small intestine involves interaction with adenylate cyclase [9012-42-4] and/or the elevation of tissue cyclic AMP [60-92-4] levels. Adenylate cyclase was prepared by

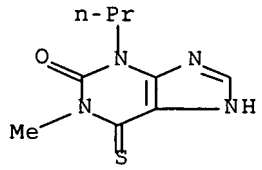
gentle homogenization of an isolated smooth muscle cell fraction obtained after collagenase digestion of longitudinal muscle strips. A number of analogs and derivs. of I possessing a primary or secondary 6-amino group inhibited the enzyme similarly to I; however, there was no correlation between compds. known to relax the intact tissue and the existence, or the degree of, cyclase inhibition. Isolated muscle strips were exposed to adrenaline bitartrate [51-42-3], DL-isoprenaline-HCl [949-36-0], I, or ATP [56-65-5], at doses causing 30-60% relaxation, for 60 s prior to sampling and anal. of cAMP content. While small increments in cAMP levels were found after administering adrenaline or isoprenaline, no change was found with I in the absence or presence of aminophylline [317-34-0] or 1-methyl-3-isobutylxanthine [28822-58-4]. Neither adenylate cyclase inhibition nor changes in cAMP levels appear to be part of the mechanism of the smooth muscle relaxant action of I or ATP.

IT **40915-18-2 42458-88-8 42458-91-3**
42458-94-6 42458-97-9 42458-98-0
42458-99-1 42459-01-8 42459-06-3
42459-07-4
RL: BIOL (Biological study)
(adenylate cyclase of intestine smooth muscle response to)

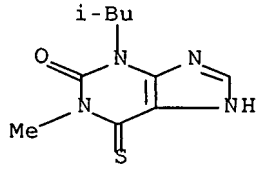
RN 40915-18-2 CAPLUS
CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



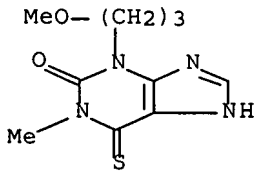
RN 42458-88-8 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



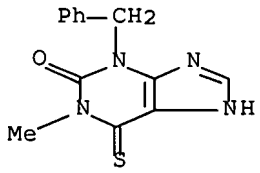
RN 42458-91-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



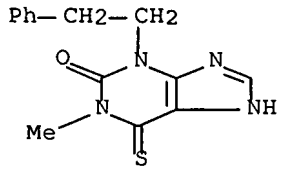
RN 42458-94-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(3-methoxypropyl)-1-methyl-6-thioxo-
(9CI) (CA INDEX NAME)



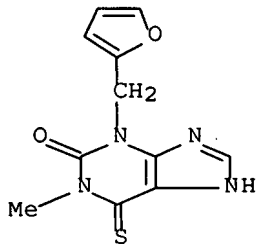
RN 42458-97-9 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(phenylmethyl)-6-thioxo-
(9CI) (CA INDEX NAME)



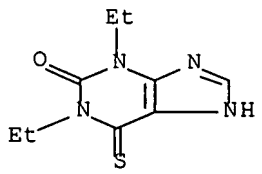
RN 42458-98-0 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-phenylethyl)-6-thioxo-
(9CI) (CA INDEX NAME)



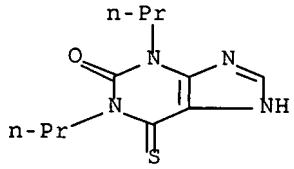
RN 42458-99-1 CAPLUS
CN 2H-Purin-2-one, 3-(2-furanylmethyl)-1,3,6,7-tetrahydro-1-methyl-6-thioxo-
(9CI) (CA INDEX NAME)



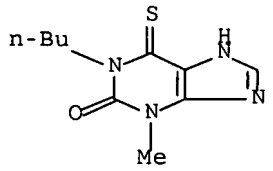
RN 42459-01-8 CAPLUS
CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



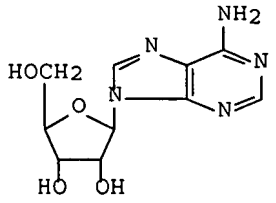
RN 42459-06-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 42459-07-4 CAPLUS
CN 2H-Purin-2-one, 1-butyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 61 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:133355 CAPLUS Full-text
DOCUMENT NUMBER: 86:133355
TITLE: Characteristics of the relaxant response of adenosine and its analogs in intestinal smooth muscle
AUTHOR(S): McKenzie, Sheila G.; Frew, Robert; Bar, Hans P.
CORPORATE SOURCE: Dep. Pharmacol., Univ. Alberta, Edmonton, AB, Can.
SOURCE: European Journal of Pharmacology (1977), 41(2), 183-92
CODEN: EJPHAZ; ISSN: 0014-2999
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI



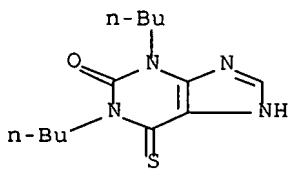
I

AB Several characteristics of the relaxant response of the isolated longitudinal muscle of the rabbit small intestine in response to the administration of adenosine (I) [58-61-7] and related compds. are studied. Following administration of I or ATP [56-65-5] the preparation responded with a rapid initial suspension of spontaneous contractile activity followed by a secondary sustained phase of inhibition of lower magnitude. Cumulative application of relaxant doses of I or ATP caused a lesser total response than that obtained by single application of the cumulative dose. Neither procaine, lidocaine or guanethidine antagonized the responses to I or ATP and the responsiveness of muscles obtained from reserpinized animals appeared unchanged. A number of I derivs. and analogs was tested for the ability to relax the muscle. Generally, compds. containing a primary or secondary 6-amino group acted as agonists with the exception of 8-bromoadenosine [2946-39-6]. Inactive nucleosides did not modify the responsiveness of the muscle to I. Responses to I and ATP were not appreciably modified by papaverine, imidazole, dipyridamole, 6-(p-nitrobenzylthio)-purine riboside. Antagonism was observed, however, with phentolamine [50-60-2] and aminophylline [317-34-0]. Aminophylline at 100 μM inhibited responses to I over a wide dose range; this antagonism was surmountable by high doses of I. 1-Methyl-3- isobutylxanthine [28822-58-4] did not antagonize I responses. A number of 1,3-alkyl-6-thioxanthines did not modify the I response at doses that did not show any direct action. The results support the concept of an extracellular receptor site of I and its analogs and the absence of an indirect mechanism of action via nerve stimulation.

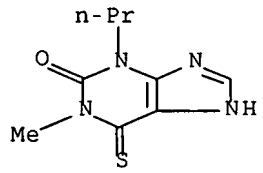
IT **40915-18-2 42458-88-8 42458-91-3 42458-94-6 42458-97-9 42458-98-0 42458-99-1 42459-01-8 42459-06-3 42459-07-4**
RL: BIOL (Biological study)
(intestine smooth muscle relaxation by adenosine and its analogs response to)

RN 40915-18-2 CAPLUS

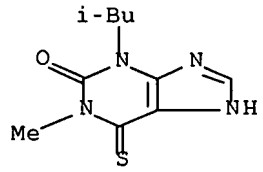
CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



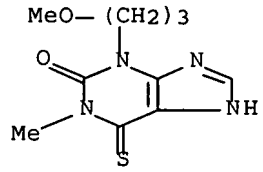
RN 42458-88-8 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



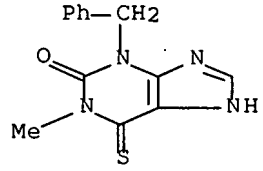
RN 42458-91-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



RN 42458-94-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(3-methoxypropyl)-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)

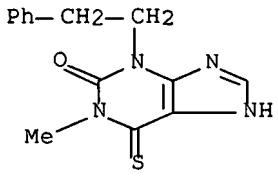


RN 42458-97-9 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(phenylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)

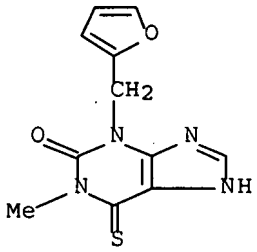


RN 42458-98-0 CAPLUS

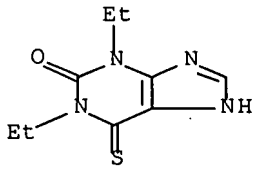
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-phenylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



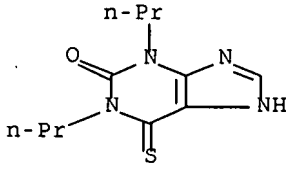
RN 42458-99-1 CAPLUS
CN 2H-Purin-2-one, 3-(2-furanylmethyl)-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 42459-01-8 CAPLUS
CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)

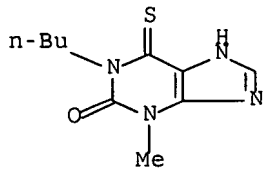


RN 42459-06-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 42459-07-4 CAPLUS

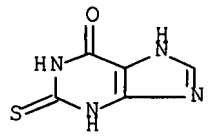
CN 2H-Purin-2-one, 1-butyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



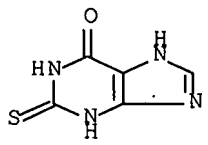
L57 ANSWER 62 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:561303 CAPLUS Full-text
DOCUMENT NUMBER: 85:161303
TITLE: Heat stabilizers for vinyl halide resins
INVENTOR(S): Sekiguchi, Tetsuo; Abe, Masami; Tsuruga, Koji; Tominaga, Nobuhide
PATENT ASSIGNEE(S): Adeka Argus Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 51088542	A	19760803	JP 1975-13797		19750131 <--
PRIORITY APPLN. INFO.:			JP 1975-13797	A	19750131 <--

ED Entered STN: 12 May 1984
AB PVC [9002-86-2] (optionally containing ABS [9003-56-9]) and poly(vinyl fluoride) [24981-14-4] contained heterocyclic compds. containing -N:C(SH)NRC(:R1)- groups (R = H, alkyl, aryl; R1 = O, S; including tautomeric forms or salts) as heat stabilizers. For example, a PVC composition containing DOP 50, epoxidized soybean oil 2, tris(nonylphenyl) phosphite 0.5, stearic acid 0.5, and 3,5-dimercapto-1,2,4-triazole (I) [5650-03-3] 0.05 phr had heat stability (175°) 60 min, compared with 30 min for a control not containing I.
IT **2487-40-3 60682-54-4**
RL: MOA (Modifier or additive use); USES (Uses)
(heat stabilizers, for vinyl halide resins)
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 60682-54-4 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo-, barium salt (1:1) (9CI) (CA INDEX NAME)

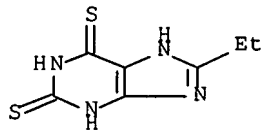


● Ba

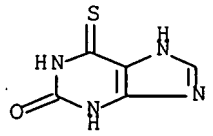
L57 ANSWER 63 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:470075 CAPLUS Full-text
DOCUMENT NUMBER: 85:70075
TITLE: Copper electroplating from pyrophosphate baths
INVENTOR(S): Nakamura, Minoru; Minagawa, Tadashi; Asai, Osamu
PATENT ASSIGNEE(S): Hitachi, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 51021529	A	19760220	JP 1974-93391		19740816 <--
PRIORITY APPLN. INFO.:			JP 1974-93391	A	19740816 <--

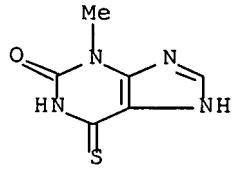
ED Entered STN: 12 May 1984
AB The formation of brittle films on Cu electroplates produced in a Cu2P2O7 bath is prevented by adding, prior to or following embrittlement, an embrittlement inhibitor 0.00001-0.1 g/l. to a plating bath with a H4P2O7/Cu ratio of 9.2-8.5. The embrittlement inhibitor was ≥1 compds. selected from mercaptopurines, mercaptopyrazineimidazoles, mercaptopyrazinethiazoles, mercaptopyridinethiazoles and their alkyl, amino, Ph, or OH derivs. Thus, Cu was plated on stainless steel in a bath containing Cu2P2O7.3H2O 70, K4P2O7 316 g/l., 27% NH4OH 5 ml/l., KNO3 15 g/l. and 2,6-dimercapto-8-ethylpurine (I) 1 mg/l. at a pH of 8.5, a bath temperature of 55°, an anode c.d. of 4.5 A/dm2, a cathode c.d. of 3.0 A/dm2, and air stirring. The formation of a brittle film did not occur up to 45-55 hr. In contrast, embrittlement occurred within 20-25 hr in the absence of I.
IT **60022-13-1**
RL: PRP (Properties)
(in electroplating, embrittlement inhibitor for copper)
RN 60022-13-1 CAPLUS
CN 1H-Purine-2,6-dithione, 8-ethyl-3,7-dihydro- (9CI) (CA INDEX NAME)



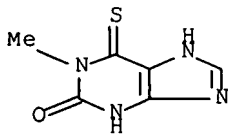
L57 ANSWER 64 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:416151 CAPLUS Full-text
DOCUMENT NUMBER: 85:16151
TITLE: Oxidation of N-methyl substituted hypoxanthines, xanthines, purine-6,8-diones and the corresponding 6-thioxo derivatives by bovine milk xanthine oxidase
AUTHOR(S): Bergmann, Felix; Levene, Lawrence
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Biochimica et Biophysica Acta, Enzymology (1976), 429(3), 672-88
CODEN: BBEZAD; ISSN: 0924-1086
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
AB The oxidation of 6 series of purines (hypoxanthines, xanthines, purine-6,8-diones, and the corresponding 6-thioxo derivs.) by a highly purified bovine milk xanthine oxidase was studied, using a variety of N-Me derivs. N-Me substituents can either enhance or reduce enzymic rates. Enhancement is ascribed to blockage of groups which mediate unfavorable modes of binding of substrate to enzyme. Introduction of N-Me groups can also inhibit enzymic oxidation, either by occluding essential binding groups or by preventing spontaneous or enzyme-induced tautomerization processes, which create suitable binding sites in the substrates. In all purines which are rapidly attacked by xanthine oxidase, proper attachment to the active center is mediated by the groupings (3)NH, (9)N, or (3)N, (9)NH. Reduced rates usually express lowered substrate affinity, which finds its expression in weak competitive inhibition of xanthine oxidation
IT **2002-59-7 33285-76-6 38695-85-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, enzymic)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



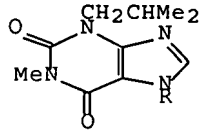
RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 38695-85-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



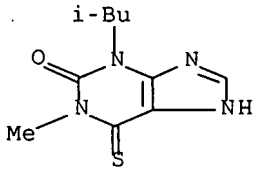
L57 ANSWER 65 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:130133 CAPLUS Full-text
DOCUMENT NUMBER: 84:130133
TITLE: Inhibition of separated forms of phosphodiesterases from pig coronary arteries by uracils and by 7-substituted derivatives of 1-methyl-3-isobutylxanthine
AUTHOR(S): Garst, J. E.; Kramer, G. L.; Wu, Y. J.; Wells, J. N.
CORPORATE SOURCE: Sch. Med., Vanderbilt Univ., Nashville, TN, USA
SOURCE: Journal of Medicinal Chemistry (1976), 19(4), 499-503
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI



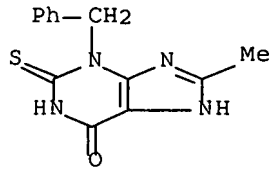
I

AB A series of 15 title xanthine derivs. (I; R = alkyl, aralkyl, alicyclicalkyl, propargyl, 4-picolyl), prepared by alkylation of 1-methyl-3-isobutylxanthine (I, R = H)(MIX) [28822-58-4] were tested for specificity of inhibition of chromatog.-separated cyclic nucleotide phosphodiesterase [50812-31-2] activity fractions I and II. I were generally much less potent than MIX as inhibitors of activity fraction II, but some retained the potency of MIX as inhibitors of activity fraction I. 1-Methyl-3-isobutyl-7-benzylxanthine (I, R = PhCH2) [58481-23-5] was 20-30 times more potent as an inhibitor of activity fraction I than of II, while retaining the potency of MIX against activity fraction I. A series of 1,3-dialkyluracils had low potency as phosphodiesterase inhibitors. Structure-activity relations were discussed.

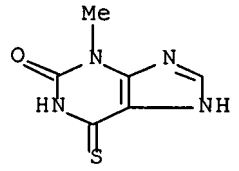
IT **42458-91-3**
RL: BIOL (Biological study)
(cyclic nucleotide phosphodiesterases inhibition by)
RN 42458-91-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 66 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:105543 CAPLUS Full-text
DOCUMENT NUMBER: 84:105543
TITLE: Thermal decomposition of quaternary hypoxanthinium salts and related purines
AUTHOR(S): Bergmann, Felix; Rahat, Miriam
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (2), 239-43
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB Addnl. data considered in abstracting and indexing are available from a source cited in the original document. Thermal decomposition of quaternary hypoxanthinium salts was achieved by heating their solns. in DMF. 1,3-Dialkylhypoxanthinium bromides or iodides lost the 3-substituent as alkyl halide, which then attacked the imidazole ring at N-7 or N-9. Thermolysis of the dioxotetrahydropurinium iodide I (R = H) involved either loss of the 3-Me group as MeI giving the dihydromethylpurinedione II (R = H), or removal of HI to give the corresponding betaine which was then methylated at N-9 to give the dioxotetrahydropurinium iodide I (R = Me). The latter compound in turn decomposed to give the dimethylpurinedione II (R = Me). Similarly, the dimethylhypoxanthinium iodide III (R = H) was degraded mainly by loss of MeI, giving IV (R = H) and small amts. of V (R = H). III (R = H) also lost HI to give the corresponding betaine, which methylated at N-1 to give III (R = Me). III (R = Me) again underwent thermolysis to give a mixture of IV (R = Me) and its 9-Me isomer.
IT **59311-65-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, reduction, and NMR of)
RN 59311-65-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-3-(phenylmethyl)-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 67 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:90117 CAPLUS Full-text
DOCUMENT NUMBER: 84:90117
TITLE: Reactions of 2-, 6-, and 8-monosubstituted 1- and 3-methylpurines with hydroxide ions in water
AUTHOR(S): Badger, Rodney J.; Barlin, Gordon B.
CORPORATE SOURCE: John Curtin Sch. Med. Res., Aust. Natl. Univ., Canberra, Australia
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (2), 151-5
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 84:90117
ED Entered STN: 12 May 1984
AB 1-Methyl-2- and 6-methylthiopurine underwent nucleophilic displacement with NaOH to give the 2- and 6-hydroxypurine analogs, resp. whereas 1-methyl-8-methylthiopurine underwent ring cleavage to give 5-amino-2-methylthioimidazole-4-carboxaldehyde. 3-Methyl-6- methylthiopurine with NaOH gave predominantly 5-methylaminoimidazole-4- carboxaldehyde, whereas 3-methyl-8-methylthiopurine underwent ring cleavage like its 1-methyl isomer. 7- And 9-methyl-2-methylthiopurines gave 4-amino-5-methylamino- and 5-amino-4-methylamino-2- methylthiopyrimidines, resp. Hydrolysis of 6-chloro-3-methylpurine gave 5-methylaminoimidazole-4-carbonitrile and some 6-hydroxy-3-methylpurine. 8-Chloro-3-methylpurine was hydrolyzed without formation of the 8-hydroxy compound
IT **33285-76-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)
RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 68 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:125358 CAPLUS Full-text
DOCUMENT NUMBER: 82:125358
TITLE: Preparation of some N-methylisoguanines via 6-methylthio-2-oxopurines, and 8-methylisoguanine
AUTHOR(S): Kazimierczuk, Z.; Shugar, D.
CORPORATE SOURCE: Inst. Exp. Phys., Univ. Warsaw, Warsaw, Pol.
SOURCE: Acta Biochimica Polonica (1974), 21(4), 455-63
CODEN: ABPLAF; ISSN: 0001-527X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 82:125358
ED Entered STN: 12 May 1984

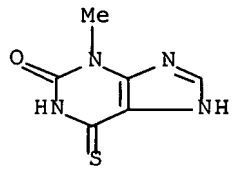
GI For diagram(s), see printed CA Issue.

AB Isoguanines I (R-R3 = H, Me) were obtained by reaction of R2R3NH with 6-methylthio-2-oxopurines, prepared by treating the xanthines with P2S5 and methylating. 8-Methylisoguanine was prepared from 4,5,6-triaminopyrimidin-2-one and AcNH2. The pK values of I and II are reported. II (R = Me, R2 = R3 = H) was resistant to HNO2 deamination, whereas I (R2 = R3 = H) were easily deaminated.

IT **33285-76-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 33285-76-6 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 69 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1974:107452 CAPLUS Full-text

DOCUMENT NUMBER: 80:107452

TITLE: Mass spectra of N- and S-methylpurines

AUTHOR(S): Deutsch, J.; Neiman, Z.; Bergmann, F.

CORPORATE SOURCE: Dep. Pharm. Chem., Hebrew Univ., Jerusalem, Israel

SOURCE: Jerusalem Symposia on Quantum Chemistry and Biochemistry (**1972**), 4, 402-11
CODEN: JSQCA7; ISSN: 0075-3696

DOCUMENT TYPE: Journal

LANGUAGE: English

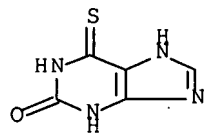
ED Entered STN: 12 May 1984

AB The mass spectra of hypoxanthines, 6-purinethiones, adenines, and 6-(methylamino)purines are given. The 7-Me derivs. of these compds. lose a H atom to give M-1 cation which is stabilized by cyclization. The analogous process occurs in 6-(methylthio)purines by loss of a H atom from the MeS group. The cyclization process is reflected by abundant metastable peaks.

IT **2002-59-7 2487-40-3 5437-25-2**
33285-76-6
RL: PRP (Properties)
(mass spectrum of)

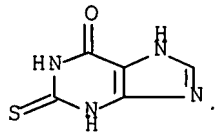
RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)

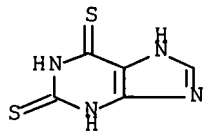


RN 2487-40-3 CAPLUS

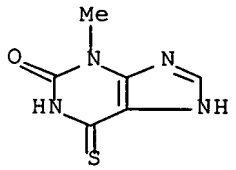
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 5437-25-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



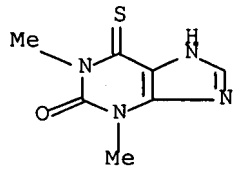
RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



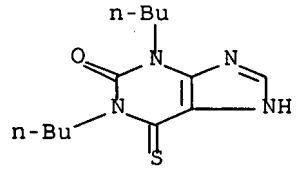
L57 ANSWER 70 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:427084 CAPLUS Full-text
DOCUMENT NUMBER: 79:27084
TITLE: Structure-activity relations. III. Bronchodilator activity of substituted 6-thioxanthines
AUTHOR(S): Bowden, Keith; Wooldridge, Kenneth R. H.
CORPORATE SOURCE: Dep. Chem., Univ. Essex, Colchester/Essex, UK
SOURCE: Biochemical Pharmacology (**1973**), 22(9), 1015-21
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
AB A correlation of the bronchodilator activity of a series of substituted 6-thioxanthines (I) was made with partition parameters and (or) the steric effect of the 1- and 3-substituents. An increase in activity was observed on introduction of bulky substituents at R3 and particularly at R1. The 3-substituted series were also correlated by a Hansch relation involving partition factors alone. Thus, 1,3-dibutyl-6-thioxanthine [**40915-18-2**] was far more active than 1,3-dimethyl-6-thioxanthine [**2398-70-1**].
IT **2398-70-1 40915-18-2 42458-87-7**

42458-88-8 42458-89-9 42458-90-2
42458-91-3 42458-92-4 42458-93-5
42458-94-6 42458-95-7 42458-96-8
42458-97-9 42458-98-0 42458-99-1
42459-00-7 42459-01-8 42459-02-9
42459-03-0 42459-04-1 42459-06-3
42459-07-4 42459-09-6 42459-10-9
RL: BIOL (Biological study)
(bronchodilator)

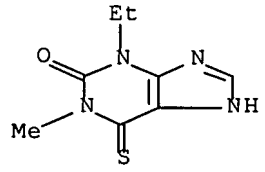
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



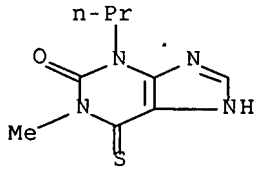
RN 40915-18-2 CAPLUS
CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



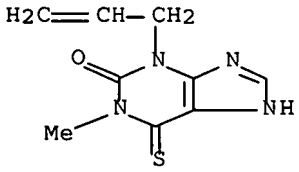
RN 42458-87-7 CAPLUS
CN 2H-Purin-2-one, 3-ethyl-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



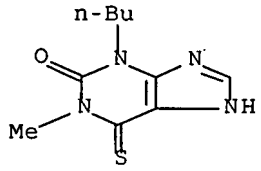
RN 42458-88-8 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-propyl-6-thioxo- (9CI) (CA INDEX NAME)



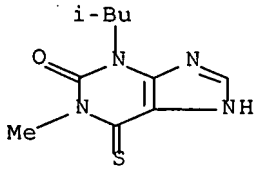
RN 42458-89-9 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-propenyl)-6-thioxo- (9CI) (CA INDEX NAME)



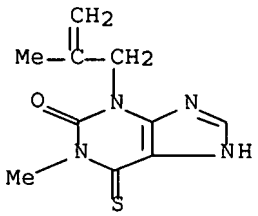
RN 42458-90-2 CAPLUS
CN 2H-Purin-2-one, 3-butyl-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



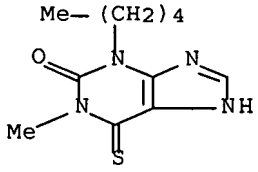
RN 42458-91-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



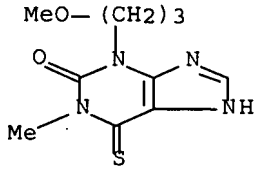
RN 42458-92-4 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methyl-2-propenyl)-6-thioxo- (9CI) (CA INDEX NAME)



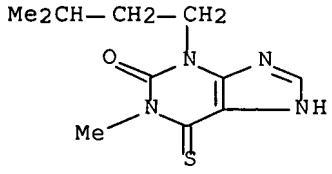
RN 42458-93-5 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-pentyl-6-thioxo- (9CI) (CA INDEX NAME)



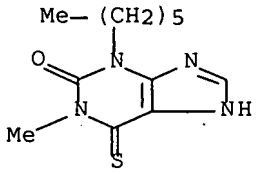
RN 42458-94-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(3-methoxypropyl)-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



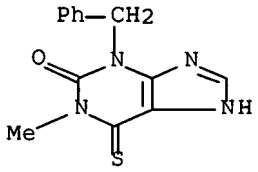
RN 42458-95-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(3-methylbutyl)-6-thioxo- (9CI) (CA INDEX NAME)



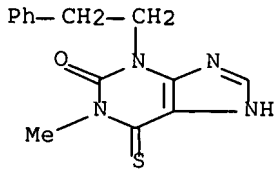
RN 42458-96-8 CAPLUS
CN 2H-Purin-2-one, 3-hexyl-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



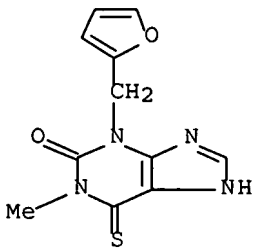
RN 42458-97-9 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(phenylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



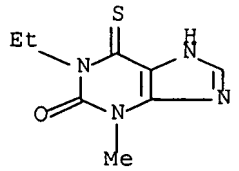
RN 42458-98-0 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-phenylethyl)-6-thioxo- (9CI) (CA INDEX NAME)



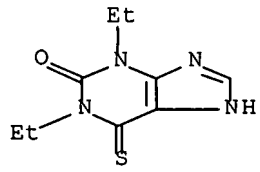
RN 42458-99-1 CAPLUS
CN 2H-Purin-2-one, 3-(2-furanylmethyl)-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



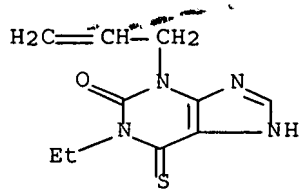
RN 42459-00-7 CAPLUS
CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



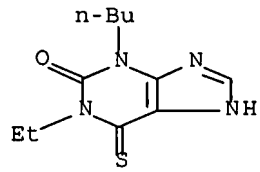
RN 42459-01-8 CAPLUS
CN 2H-Purin-2-one, 1,3-diethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



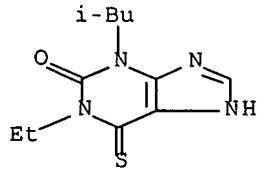
RN 42459-02-9 CAPLUS
CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-(2-propenyl)-6-thioxo- (9CI) (CA INDEX NAME)



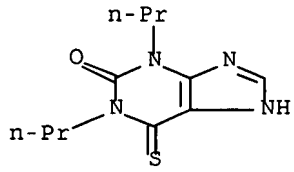
RN 42459-03-0 CAPLUS
CN 2H-Purin-2-one, 3-butyl-1-ethyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



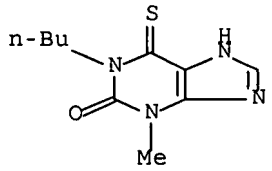
RN 42459-04-1 CAPLUS
CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



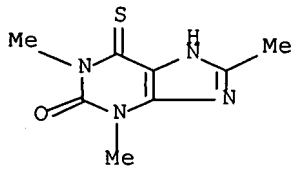
RN 42459-06-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo- (9CI) (CA INDEX NAME)



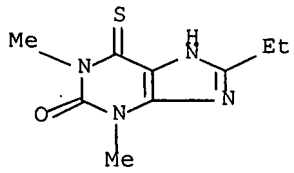
RN 42459-07-4 CAPLUS
CN 2H-Purin-2-one, 1-butyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



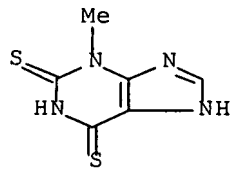
RN 42459-09-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3,8-trimethyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 42459-10-9 CAPLUS
CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 71 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:136229 CAPLUS Full-text
DOCUMENT NUMBER: 78:136229
TITLE: Tautomerism, protonation, and methylation in (methylthio)purines. Factors determining electrophilic attack on purines
AUTHOR(S): Reichman, Uri; Bergmann, Felix; Lichtenberg, Dov; Neiman, Zohar
CORPORATE SOURCE: Dep. Pharmacol., Heb. Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1973), No. 8, 793-800
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
AB The predominant tautomers, the position of protonation in aqueous solution, and the course of methylation in aprotic solvents were determined for all the mono- and bis(methylthio)purines and for 2,6,8,-tis(methylthio)purine. Protonation gave resonating cations in which the charge is distributed over both rings. 8-(Methylthio)-and 2,8-bis(methylthio)purine underwent methylation at N-1. 6-(Methylthio)-, 6,8-bis(methylthio)-, and 2,6,8-tris(methylthio)purine gave N-3 Me derivs. Methylation of 2-(methylthio)- and 2,6-bis(methylthio)purine occurred at both N-7 and N-9. The results were explained in terms of electronic and steric factors
IT **33285-77-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation of)
RN 33285-77-7 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)

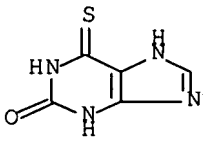


L57 ANSWER 72 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:72173 CAPLUS Full-text
DOCUMENT NUMBER: 78:72173
TITLE: Cephalosporins
INVENTOR(S): Sugimoto, Keiichi; Kobayashi, Kunio; Nishijima, Kouji; Morimoto, Shiro
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd.

SOURCE: Ger. Offen., 43 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2225694	A	19721214	DE 1972-2225694	19720526 <--
DE 2225694	B2	19750410		
DE 2225694	C3	19751120		
JP 51016436	B	19760524	JP 1971-38007	19710531 <--
AU 7242504	A	19731122	AU 1972-42504	19720519 <--
ES 403305	A1	19750501	ES 1972-403305	19720530 <--
BE 784181	A1	19721130	BE 1972-4069	19720531 <--
NL 7207368	A	19721204	NL 1972-7368	19720531 <--
FR 2140133	A1	19730112	FR 1972-19538	19720531 <--
HU 164340	B	19740128	HU 1972-TA1189	19720531 <--
GB 1348737	A	19740320	GB 1972-25417	19720531 <--
AT 316746	B	19740725	AT 1972-4720	19720531 <--
AT 318810	B	19741125	AT 1973-4101	19720531 <--
US 3872115	A	19750318	US 1972-258177	19720531 <--

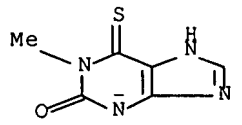
PRIORITY APPLN. INFO.: JP 1971-38007 A 19710531 <--
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB 3-(Heterocyclic methyl)ceph-3-em derivs. [I; R = 5-R2-6-R3-1,2-dihydro-2- oxo-4-pyrimidinyl (R2 = H, NH2, Me, OH, CO2H, R3 = H, OH, NMe2, CO2H), 2-oxopurin-6-yl; R1 = PhCHR4 (R4 = H, NH2, HO3S, HO, H2NCO), cyclohexylmethyl, PhSCH2, 1-tetrazolylmethyl, EtCHBr, NCCH2, PhOCH2] were prepared by treating the corresponding cephalosporanic acid with a heterocyclic mercaptol. Thus, Na 7-(2-thienylacetamido)cephalosporanate was treated with 4-thiopyrimidin-2-one in Me2SO to give I (R = 1,2-dihydro-2-oxo-4-pyrimidinyl, R1 = 2-thienyl).
IT **39879-29-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sodium acetoxymethyl(thienylacetamido)cephalosporanate)
RN 39879-29-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo-, monoammonium salt (9CI) (CA INDEX NAME)



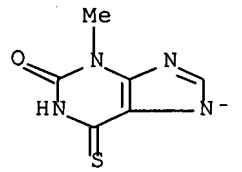
● NH_3

L57 ANSWER 73 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:513624 CAPLUS Full-text
DOCUMENT NUMBER: 77:113624
TITLE: Tautomerism and ionization processes in 6-thioxanthine and its N-methyl derivatives

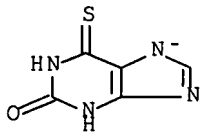
AUTHOR(S): Lichtenberg, D.; Bergmann, F.; Neiman, Z.
CORPORATE SOURCE: Dep. Pharm., Heb. Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (**1972**), (11), 1676-81
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB Uv and PMR spectra were recorded of 6-thioxanthine and 10 of its N-Me derivs.; spectra were also obtained of some of their mono- and dianionic and cationic forms. In aqueous solns. of thioxanthines with a free NH in the imidazole ring the 7-NH-tautomer (I) predominated. The order of NH-group acidities was 3 > 7 > 1. The anions of 6-thioxanthine and its 1-Me derivative tautomerized to the NH form. Interactions between H and Me groups at positions 3 and 9 were indicated by the pK values of the 9-methylthioxanthines and by the large downfield displacement of the PMR signals of the 3- and 9-Me groups in 3,9-dimethylthioxanthines.
IT **38759-09-0 38759-10-3 38759-11-4**
38759-12-5 38759-18-1 38759-19-2
38800-21-4 38814-97-0 38814-98-1
38814-99-2 38887-43-3
RL: PRP (Properties)
(NMR and uv spectrum of)
RN 38759-09-0 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo-, ion(1-) (9CI) (CA INDEX NAME)



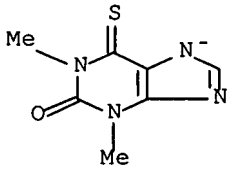
RN 38759-10-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo-, ion(1-) (9CI) (CA INDEX NAME)



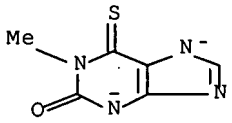
RN 38759-11-4 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo-, ion(1-) (9CI) (CA INDEX NAME)



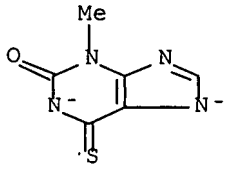
RN 38759-12-5 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo-, ion(1-) (9CI) (CA INDEX NAME)



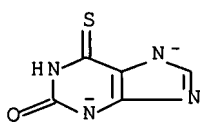
RN 38759-18-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo-, ion(2-) (9CI) (CA INDEX NAME)



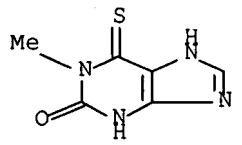
RN 38759-19-2 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo-, ion(2-) (9CI) (CA INDEX NAME)



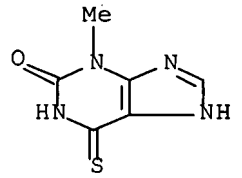
RN 38800-21-4 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo-, ion(2-) (9CI) (CA INDEX NAME)



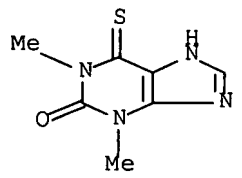
RN 38814-97-0 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo-, conjugate monoacid (9CI) (CA INDEX NAME)



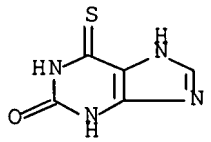
RN 38814-98-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo-, conjugate monoacid (9CI) (CA INDEX NAME)



RN 38814-99-2 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo-, conjugate monoacid (9CI) (CA INDEX NAME)

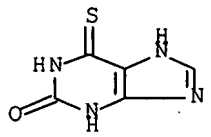


RN 38887-43-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo-, conjugate monoacid (9CI) (CA INDEX NAME)

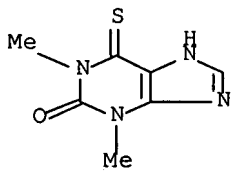


IT **2002-59-7 2398-70-1 33285-76-6**
38695-85-1
RL: PRP (Properties)
(ionization and tautomerism of)

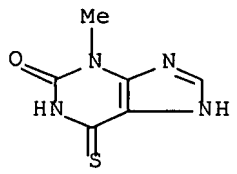
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



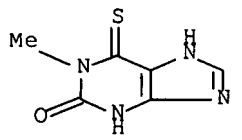
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



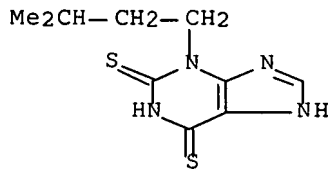
RN 38695-85-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 74 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:493013 CAPLUS Full-text
DOCUMENT NUMBER: 75:93013
TITLE: Photographic silver halide materials supersensitized with a combination of a triazole and a cyanine dye
INVENTOR(S): Brooks, Dugald A.
PATENT ASSIGNEE(S): Eastman Kodak Co.
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

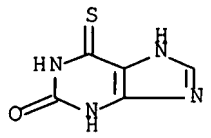
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3592656	A	19710713	US 1968-757147	19680903 <--
BE 738386	A	19700216	BE 1969-738386	19690903 <--
FR 2020524	A5	19700717	FR 1969-29985	19690903 <--
GB 1282032	A	19720719	GB 1969-1282032	19690903 <--

PRIORITY APPLN. INFO.: US 1968-757147 A 19680903 <--
ED Entered STN: 12 May 1984
AB Photog. Ag halide emulsions were supersensitized by a combination of a sensitizing methine dye and pyrazolone, triazole, tetrazole, or imidazole. For example, a Ag(Br,I) emulsion containing 80 mg 3,3'-diethyl-4,5,4',5'-naphthoselenadicarbocyanine iodide/mole Ag and 0.3-10g 3-(3,4-dichloroanilino)-1-(2,4,6-trichlorophenyl)-5-pyrazolone/mole Ag was exposed and gave a relative speed 692 compared to 100 for a similar emulsion containing no pyrazolone.
IT **32051-91-5**
RL: USES (Uses)
(photographic supersensitizers from cyanine dyes and)
RN 32051-91-5 CAPLUS
CN Xanthine, 3-isopentyl-2,6-dithio- (7CI, 8CI) (CA INDEX NAME)

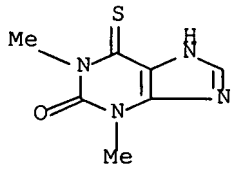


L57 ANSWER 75 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:434696 CAPLUS Full-text

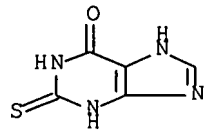
DOCUMENT NUMBER: 75:34696
TITLE: Nuclear magnetic resonance spectra of xanthines and thioxanthines
AUTHOR(S): Bergmann, F.; Lichtenberg, D.; Neiman, Z.
CORPORATE SOURCE: Hadassah Med. Sch., Heb. Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (10), 1939-41
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
AB The NMR signal of the 8-H in xanthines is shifted downfield more strongly by introduction of a 2- than of a 6-thioxo group. The signals of N-Me groups are also shifted to lower field, but the effect depends strictly on the distance between the Me and the thioxo. In 2-thioxanthines, the displacement decreases in the order 1-Me = 3-Me > 7-Me, and in 6-thioxanthines the sequence is 1-Me > 7-Me > 3-Me > 9-Me.
IT **2002-59-7 2398-70-1 2487-40-3**
5437-25-2 6501-94-6 6603-63-0
28139-02-8 33285-76-6 33285-77-7
RL: PRP (Properties)
(nuclear magnetic resonance of)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



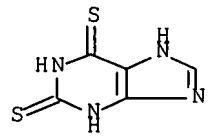
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



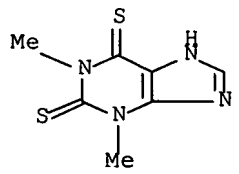
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



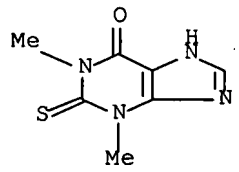
RN 5437-25-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



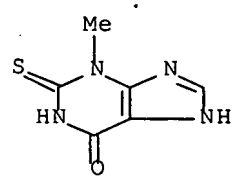
RN 6501-94-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



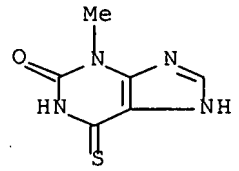
RN 6603-63-0 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



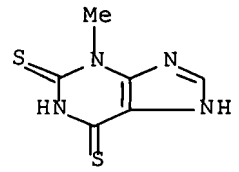
RN 28139-02-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



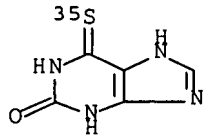
RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 33285-77-7 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



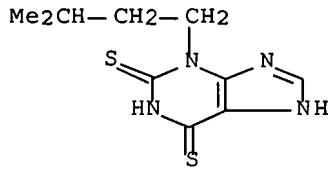
L57 ANSWER 76 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:125639 CAPLUS Full-text
DOCUMENT NUMBER: 74:125639
TITLE: Sulfur-35 labeling of some organic compounds by a dry method
AUTHOR(S): Chiotan, Constantin; Zamfir, Ioana; Szabo, Maria; Turcanu, Cornelius N.
CORPORATE SOURCE: Inst. At. Phys., Bucharest, Rom.
SOURCE: Nov. Metody Poluch. Radioaktiv. Prep., Sb. Dokl. Simp. (1970), Meeting Date 1969, 386-401. Postoyan. Kom. Ispol'z. At. Energ. Mirnykh Tselyakh: Warsaw, Pol.
CODEN: 22YYAY
DOCUMENT TYPE: Conference
LANGUAGE: Russian
ED Entered STN: 12 May 1984
AB The S in p-AcNHC6H4CH:NNHCSNH2, (H2N)2CS, PhNHCSNH2, 6-mercaptopurine, and 2-thioxanthine was replaced with 35S by heating at 150-280° with excess elemental 35S. 6-Thioguanine-35S was prepared from the unlabeled compound by acetylation, isotope exchange as above, and hydrolysis. 2-Thiouracil and its 6-Me derivative were labeled by heating at 200 and 250°, resp., with equal quantities of 35S and C10H8; MeC35SNH2 was prepared by this method in refluxing iso-BuOH. Heating sulfanilamide at 180° with (NH4)235SO4 afforded p-H2NC6H435SO2NH2.
IT **31494-01-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 31494-01-6 CAPLUS
CN Xanthine, 6-thio-35S- (8CI) (CA INDEX NAME)



L57 ANSWER 77 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:118381 CAPLUS Full-text
DOCUMENT NUMBER: 74:118381
TITLE: Silver halide photographic emulsions containing supersensitizing compositions
INVENTOR(S): Brooks, Dugald Arthur
PATENT ASSIGNEE(S): Eastman Kodak Co.
SOURCE: Fr. Demande, 21 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

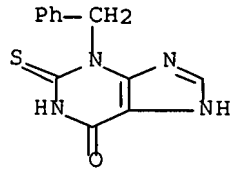
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2020524	A5	19700717	FR 1969-29985	19690903 <--
US 3592656	A	19710713	US 1968-757147	19680903 <--

PRIORITY APPLN. INFO.: US 1968-757147 A 19680903 <--
ED Entered STN: 12 May 1984
AB The title emulsions contain a sensitizing dye in conjunction with a heterocyclic compound such as 5-pyrazolone, 1,2,3,4-tetrazole, 1,2,4-triazole, imidazole, or an imidazolinium salt. E.g., a gelatin Ag(Br,I) (0.77 mole % AgI) emulsion was combined with 80 mg 5-[bis[1-ethyl-2(1H)-β - naphthothiazolylidene]isopropylidene] - 1,3 - bis(β - methoxyethyl)barbituric acid per mole Ag halide and with 0.66 g 1,5-diphenyl-1,2,4-triazole (I) per g atom Ag. The emulsion was ripened for 10 min at 50°, coated on a cellulose acetate support to give 46 mg Ag/dm2, and sensitometrically tested. A similar material without I was tested for comparison. The relative sensitivity of both materials was 75,900 and 100, resp., γ 1.50 and 1.33, and fog 0.06 and 0.05.
IT **32051-91-5**
RL: USES (Uses)
(photographic supersensitizers from carbocyanine dyes and)
RN 32051-91-5 CAPLUS
CN Xanthine, 3-isopentyl-2,6-dithio- (7CI, 8CI) (CA INDEX NAME)



L57 ANSWER 78 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:466537 CAPLUS Full-text

DOCUMENT NUMBER: 73:66537
TITLE: N .far. N alkyl and glycosyl migration of purines and pyrimidines. III. N .far. N alkyl and glycosyl migration of purine derivatives
AUTHOR(S): Miyaki, Michiko; Shimizu, Bunji
CORPORATE SOURCE: Cent. Res. Lab., Sankyo Co., Ltd., Tokyo, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1970), 18(7), 1446-56
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 73:66537
ED Entered STN: 12 May 1984
AB Alkyl and glycosyl migration reactions of N1-, N3-, N7-, and N9-substituted derivs. of adenine, N6,N6-dimethyladenine, N2-acetylguanine, and purine were demonstrated. The NMR chemical shifts of these derivs. were determined and the frontier π-electron ds. of nitrogens in purine ring calculated by a simple LCAOMO method. The results provided the order of thermodynamic stability and kinetic effect of the derivs. on the alkylation reaction.
IT **28741-76-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 28741-76-6 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-(phenylmethyl)-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 79 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:444460 CAPLUS Full-text
DOCUMENT NUMBER: 73:44460
TITLE: Charge transfer spectra of bases, nucleosides, and nucleotides
AUTHOR(S): Saucin, Michel; Van de Vorst, Albert
CORPORATE SOURCE: Dep. Phys. At. Mol., Univ. Liege, Sart-Tilman/Liege, Belg.
SOURCE: Journal de Chimie Physique et de Physico-Chimie Biologique (1970), 67(3), 507-11
CODEN: JCPBAN; ISSN: 0021-7689
DOCUMENT TYPE: Journal
LANGUAGE: French
ED Entered STN: 12 May 1984
AB Spectrophotometric investigation was carried out in systems formed by purines, pyrimidines, nucleosides, and nucleotides as donors and chloranil and 1,3,5-trinitrobenzene as acceptor. In some cases, a partial charge transfer is observed which manifests itself by the appearance of a new optical band, but, in general, specific bands of the acceptor's ion were observed, which can be interpreted as the complete transfer of an electron. Most of the mols. are very good electron donors.
IT **29373-31-7 29665-67-6**

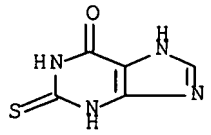
RL: PRP (Properties)
(spectrum of, uv, charge-transfer band in)

RN 29373-31-7 CAPLUS

CN p-Benzoquinone, 2,3,5,6-tetrachloro-, compd. with 2-thioxanthine (8CI) (CA INDEX NAME)

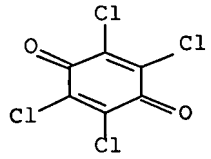
CM 1

CRN 2487-40-3
CMF C5 H4 N4 O S



CM 2

CRN 118-75-2
CMF C6 Cl4 O2

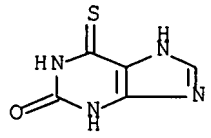


RN 29665-67-6 CAPLUS

CN p-Benzoquinone, 2,3,5,6-tetrachloro-, compd. with 6-thioxanthine (8CI) (CA INDEX NAME)

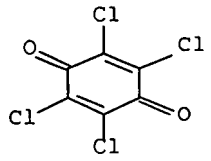
CM 1

CRN 2002-59-7
CMF C5 H4 N4 O S

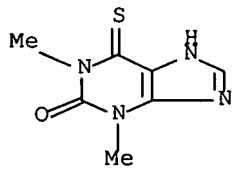


CM 2

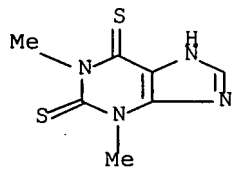
CRN 118-75-2
CMF C6 Cl4 O2



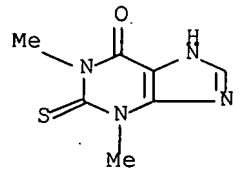
L57 ANSWER 80 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:403341 CAPLUS Full-text
DOCUMENT NUMBER: 73:3341
TITLE: Dipole moments and electronic structure of some xanthine and thioxanthine derivatives
AUTHOR(S): Weiler-Feilchenfeld, Hannah; Neiman, Zohar
CORPORATE SOURCE: Dep. Org. Chem., Hebrew Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society [Section] B: Physical Organic (1970), 4, 596-8
CODEN: JCSPAC; ISSN: 0045-6470
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
AB The dipole moments and uv absorption spectra of caffeine, theophylline, and their 2-thio-, 6-thio- and 2,6-dithio derivs. were measured. From the differences between the moments of these compounds it can be deduced that the C:S group moment is higher by 1.1 D than that of C:O; the direction of the moment of caffeine forms an angle of 96° counterclockwise with the C(4) → C(5) axis, in good agreement with theoretical predictions.
IT **2398-70-1 6501-94-6 6603-63-0**
RL: PRP (Properties)
(dipole moment of)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



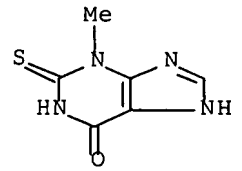
RN 6501-94-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 6603-63-0 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)

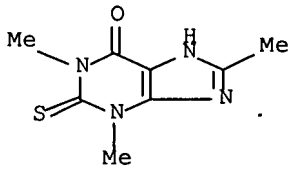


L57 ANSWER 81 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:126337 CAPLUS Full-text
DOCUMENT NUMBER: 72:126337
TITLE: Mass spectrometric investigations of heterocyclic compounds. V. Fragmentation of some purines
AUTHOR(S): Heiss, Juergen; Zeller, Klaus P.; Voelter, Wolfgang
CORPORATE SOURCE: Chem. Inst., Univ. Tuebingen, Tuebingen, Fed. Rep. Ger.
SOURCE: Organic Mass Spectrometry (1970), 3(2), 181-90
CODEN: ORMSBG; ISSN: 0030-493X
DOCUMENT TYPE: Journal
LANGUAGE: German
ED Entered STN: 12 May 1984
AB The mass spectra of 9 purines are discussed. The xanthine purines eliminate HNCO and CO consecutively, whereas 3-methylhypoxanthine loses HCN and CO. In the case of 3-methylxanthine, an ion is formed whose stabilization by rearrangement is discussed. The fragmentation patterns of 3-methyl-2-thioxanthine and 3-methylthiohypo xanthine are different from those of the corresponding O analogs. 6-(Methylthio)purine and 6-methoxypurine eliminate HCS· or HCO ·, resp. For the latter reaction a mechanism is suggested.
IT **28139-02-8**
RL: PRP (Properties)
(mass spectrum of)
RN 28139-02-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 82 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1968:496632 CAPLUS Full-text
DOCUMENT NUMBER: 69:96632
TITLE: Reactions of 4,5-diaminouracils with β-oxoesters
AUTHOR(S): Stahl, P. H.; Merz, K. W.

CORPORATE SOURCE: Univ. Freiburg/Br., Freiburg/Br., Fed. Rep. Ger.
SOURCE: Pharmazie (1967), 22(11), 630-4
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: German
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB 5,6-Diamino-1,3-dimethyluracil (I) refluxed with an equimol. amount of AcCH2CO2Et gave 80% II (X = Y = O, R = Me), decompose 216-19°; 2,4-dinitrophenylhydrazone m. 255-8°. Following II were prepared (X, Y, R, m.p., m.p. after resolidification, and m.p. of 2,4- dinitrophenylhydrazone given): O, O, Ph, 250-2°, 310-40°, 268-70°; O, O, 4-O2NC6H4, 259-63°, 360°, -; O, O, pyridin-3-yl, 260-3°, 245°, 261-2°; O, O, α-furyl, 224-32°, -, -; O, S, Me, 225-8°, -, -; S, S, Me, 212°, -, -; O, S, Ph, 223-9°, -, -; S, O, pyridin-3-yl, 257-63°, -, -; O, S, pyridin-3-yl, 244-53°, -, -; S, O, 4-O2NC6H4, 230-5°, 290-300°, -; O, S, 4-O2NC6H4, 240-2°, -, -; S, S, 4-O2NC6H4, 225°, -, -. 1,3-Dimethyl-4,5-diamino-2-thiouracil (3.7 g.) and 2.6 g. AcCH2CO2Et refluxed in xylene 5 hrs. gave 86% 2,3,6,7,8,9-hexahydro-4,6,8-trimethyl-7- thio-2,9-dioxo-1H-pyrimido[4,5b] - 1,5-diazepine, m. 240-90°, which was converted into 1,3-dimethyl-4-amino-5-(acetoacetylamino)-2-thiouracil; 2,4-dinitrophenylhydrazone m. 245-7°. Also prepared was 1.3-dimethyl-4-amino-5-(1-ethoxycarbonyl-2-propylideneamino)-2-thiouracil, m. 210-22° (after resolidification m. 320-30°), which, heated to 250° and treated with NaOH gave 44% 8-methyl-2- thiotheophylline, m. 340-3°. I (2.55 g.) refluxed with 10 g. AcCH2CO2Et in 100 ml. PhNO2 gave 45.4% 8-methyltheophylline, m. 330°; picrate m. 282-305°.
IT **19673-55-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19673-55-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3,8-trimethyl-2-thioxo- (9CI) (CA INDEX NAME)



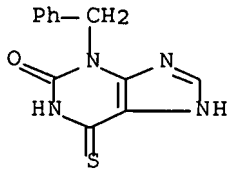
L57 ANSWER 83 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1968:459201 CAPLUS Full-text
DOCUMENT NUMBER: 69:59201
TITLE: Selective removal of the benzyl group from position 3 of purines
AUTHOR(S): Neiman, Z.; Bergmann, F.
CORPORATE SOURCE: Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SOURCE: Israel Journal of Chemistry (1968), 6(1), 9-16
CODEN: ISJCAT; ISSN: 0021-2148
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.

AB 3-Benzyl-7-methyl-6-thiopurine (I) is treated with HBr to give 7-methyl-6-thiopurine (II). Also prepared are 3-benzyl-2-thiouric acid (III) and IV. Thus, a mixture of 1 g. 3-benzyl-6-(methylthio)purine, 50 ml. MeCN, and 10 ml. MeI is refluxed 1 hr. to give 60% I, m. 220-5° (decomposition). A mixture of 1 g. 1-benzyl-5,6-diamino-4-hydroxy-2- thiopyrimidine and 3 g. urea is heated 30 min. at 180° to give III, m. >300° (HOAc); a mixture of 10 g. III, 700 ml. 3% NH3, and 100 g. Raney Ni is refluxed 2 hrs. to give 56% 3-benzyl-6,8-dihydroxypurine [IV (R = CH2Ph)] (V), m. >280° (HOAc). Similarly prepared is 3-benzyl-2-oxopurine, m. >240° (decomposition) (MeCN). A solution of 0.5 g. 3-benzyl-2-thioxanthine in 10N NaOH is heated to 50° and 1.5 ml. 30% H2O2 is slowly added to give 41% 3-benzylxanthine (VI), m. >300° (decomposition); a mixture of 1 g. VI, 3 g. P2S5, and 100 ml. pyridine is refluxed 4 hrs. to give 75% 3-benzyl-6-thioxanthine, m. >250° (decomposition). Uv data are given. Solns. of 1 g. I (and V) in 30 ml. 48% HBr are boiled 3-5 min. to give 75-90% II and IV (R = H).

IT **19844-94-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19844-94-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(phenylmethyl)-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 84 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:403051 CAPLUS Full-text
DOCUMENT NUMBER: 67:3051
TITLE: 6-Thioxanthines
AUTHOR(S): Seyden-Penne, Jacqueline; Le Thi Minh; Chabrier, Pierre
CORPORATE SOURCE: Fac. Med., Inst. Pharmacol., Paris, Fr.
SOURCE: Bulletin de la Societe Chimique de France (**1966**), (12), 3934-38
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 67:3051
ED Entered STN: 12 May 1984

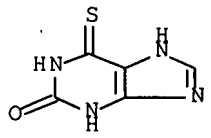
AB The reaction of 6-thiotheophyllines (I) with alkyl halides in different solvents has been examined Dry Na theophyllinate refluxed in anhydrous EtOH with an equimol. quantity of 2-chloro- and 2-bromoethanol gave a precipitate of the alkaline metal halide; on cooling the I crystallizes. In anhydrous HCONMe2 in the presence of NaH or K2CO3, only gums or the original material were obtained, depending on the temperature and reaction time. I and epoxide, in the presence of C5H5N, refluxed in anhydrous PrOH gave 7-(β-alkyl-β-hydroxyethyl)-6-thiotheophyllines in poor yields. By replacing PrOH by HCONMe2, an aprotic polar solvent which favors anionic nucleophilic substitution, the yields were appreciably increased. Thus, I (0.05 moles), 2 ml. C5H5N, and 80 ml. HCONMe2 in which were dissolved 0.125 moles ethylene oxide, kept 3 hrs. at 100° in a sealed tube, gave 50% 7-(β-hydroxyethyl)-6-

thiotheophylline, m. 137°. 7-(β-Hydroxypropyl)-6-thiotheophylline, m. 165°, 7-(β,γ-dimethoxypropyl)-6-thiotheophylline, m. 137°, and 7-(γ-chloro-β-hydroxypropyl)-6-thiotheophylline, m. 175° were similarly prepared in 50-60% yields. The structure of these compds. was confirmed by uv, ir, and N.M.R. spectra. Desulfurization of these compds. was confirmed by uv, ir, and N.M.R. spectra. Desulfurization of these compds. was accomplished using Raney Ni, rich in H, freshly prepared at temps. below 60°, by refluxing in EtOH at 96° and renewing the catalyst every hr. Thus, the following 1,3-dimethyl-2-oxo-7-alkyl-1,2,3,6-tetrahydropurines were obtained (alkyl group and m.p. given): CH2CH2OH, 210°; CH2CHOHCH3, 224°, CH2CHOHCH2OH, 240°. The uv, ir, and N.M.R. spectra of the desulfurized compds. were examined and compared to those of the alkylated I.

IT **2002-59-7DP**, Xanthine, 6-thio-, derivs. **2398-70-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

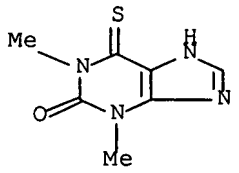
RN 2002-59-7 CAPLUS

CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



RN 2398-70-1 CAPLUS

CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 85 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1967:2448 CAPLUS Full-text

DOCUMENT NUMBER: 66:2448

TITLE: Oxidation products of thiocarboxylic acid amides. XII. Oxidation reactions of thiolimide esters and N-heteroaromatic compounds with α- and γ-thiocarbonyl groups

AUTHOR(S): Walter, Wolfgang; Voss, Juergen; Curts, Julius

CORPORATE SOURCE: Univ. Hamburg, Hamburg, Germany

SOURCE: Justus Liebigs Annalen der Chemie (1966), 695, 77-86
CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 66:2448

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

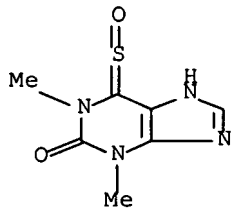
AB cf. CA 65, 13501a. Thiolimide esters 4-R1C6H4C(SR3):NC6H4R2-4 (I) are oxidized by BzOOH to the corresponding amides 4-R1C6H4CONHC6H4R2-4 (R1 and R2 same as in I) (II). 2- (III) and 4-pyridinethione (IV) and purine-6-thione (V) give with H2O2 S-oxides, which however easily react further to give disulfides, and in basic medium to give sulfonic acids. Oxidns. of other N-heteroaromatic compds. are reported. An EtOH solution of the appropriate Na thiophenolate treated with an equivalent amount appropriate imide chloride in Et2O, after 12 hrs. at room temperature the solution filtered and evaporated, and the residue recrystd. from EtOH gave .apprx.50% I. The following were prepared (R1, R2, R3, m.p., m.p. corresponding II (R1 and R2 same as in I) given): H, H, Me, 63-4°, 165-6°; H, H, Ph (VI), 54-6°, 165-6°; H, H, C6H4NO2-4 (VII), 81-4°, 165-6°; H, NO2, Ph, 108-9°, 201-2°; NO2, H, Ph, 67-8°, 213-15°; H, OMe, Ph, 64-5°, 155-7°; MeO, H, Ph, 65-6°, 175-6°; MeO, OMe, Ph, 95-6°, 204°; MeO, OMe, C6H4NO2-4, 129-31°, 204°. The appropriate I (0.1 mole) and 0.2 mole 30% H2O2 were dissolved in CHCl3 under external cooling, after 12 hrs. at room temperature, the precipitate (A) filtered off, the filtrate washed with aqueous NaHCO3, dried, and evaporated, and the residue recrystd. from EtOH with C to give the corresponding II, m.ps. being shown in the first table; in 2 cases (VI and VII) the precipitate A was identified as (PhNH3)+(O3SC6H4R)- (VIII) (R = H) and VIII (R = NO2), resp. 2-Benzylsulfinylpyridine (IX) [obtained from 2-benzylthiopyridine (X)] (1.17 g.) in 35 cc. CHCl3 kept 70 hrs. at room temperature with 0.87 g. BzOOH and the solution washed with aqueous Na2CO3, dried, and evaporated gave 0.78 g. 2-benzylsulfonylpyridine (Xa), m. 114-15° (EtOAc-petr. ether). X N-oxide (0.50 g.) and 0.34 g. BzOOH in 15 cc. CHCl3 kept 3 days at room temperature and worked up like Xa gave 0.30 g. IX N-oxide (XI), m. 119° (EtOAc-petr. ether). XI (0.47 g.) and 0.7 g. BzOOH in 15 cc. CHCl3 kept 2 days at room temperature and worked up like Xa gave 0.35 g. Xa N-oxide, m. 126-8° (EtOAc-petr. ether). 2-Thiazolidinethione (XII) (3 g.) in 150 c.. MeOH and 150 cc. CH2Cl2 treated with 2 cc. 30% H2O2 at room temperature, the solution kept 30 min. and poured into H2O, the aqueous layer separated, extracted twice with CH2Cl2, and treated dropwise with 1.5% MeOHFeCl3 (the aqueous layer was colored deep blue), and the product extracted immediately with CH2Cl2 gave 310 mg. Fe(III) complex (XIII) of XIV, blue, m. 70.5-2.0°; thin layer chromatography (TLC) on silica gel G with 3:1 C6H6-MeOH showed that XIII still contained XII. Similar oxidation of 2-oxazolidinethione gave an aqueous solution of XV, which was detected only in solution with FeCl3 (blue color). III (200 mg.) in 10 cc. CHCl3 and 5 cc. EtOH treated with 0.5 cc. 30% H2O2 and the yellow solution treated with 1% EtOH-FeCl3 gave a blue green color [indicative of III S-oxide (XVI)], which rapidly faded; after 15 min. XVI was no longer detectable. Treatment of 200 mg. IV in 10 cc. HCONMe2 (DMF) with 1 cc. 30% H2O2 gave the same result as with III. N-Methyl-2-pyridinethione (XVIa) (200 mg.) in 10 cc. CHCl3 and 10 cc. EtOH treated with 0.12 cc. 30% H2O2 and then with FeCl3 gave an olive green-blue color; on TLC on silica gel with EtOAc, the FeCl3-pos. substance remained at the starting point. III (6.7 g.) in 100 cc. MeOH kept 40 min. with 7.2 cc. 30% H2O2 and evaporated gave 4.8 g. bis(2-pyridyl) disulfide, m. 57° (6:7 C6H6-petr. ether); picrate m. 119° (EtOH). IV (200 mg.) in 10 cc. DMF kept 1 hr. with 0.5 cc. 30% H2O2 and diluted with H2O deposited 0.1 g. bis(4-pyridyl) disulfide, m. 77° (6:7 C6H6-petr. ether); picrate m. 225° (decomposition) (DMF). XVIa (100 mg.) in 3 cc. MeOH treated with 0.2 cc. Et3N and 0.3 cc. 30% H2O2, kept 5 min., and examined by TLC (silica gel, EtOAc) showed the presence of XVIa (Rf 0.41), XVIa S-oxide (Rf 0.00), and N-methyl-2-pyridone (Rf 0.10), which could be detected with iodine-azide reagent and with FeCl3 (red color). III (1.1 g.) in 50 cc. 2N NaOH kept 50 min. with 5% 30% H2O2, acidified with 2N HCl, neutralized with aqueous NaHCO3, and evaporated, the residue extracted with boiling MeOH, and the extract evaporated gave 1.25 g. Na 2-pyridine-sulfonate (XVII), m. >300° (EtOH-H2O), identical (ir spectrum) with authentic XVII. From IV was similarly obtained 11% Na 4-pyridinesulfonate (XVIII), m. >300°, identical (ir spectrum) with authentic XVIII. XVIa (0.25 g.) in 25 cc. CHCl3 and 25 cc.

EtOH heated 10 min. at 50° with 1 cc. 30% H2O2 and evaporated and the residual sirup kept 3 days at -20° gave 10 mg. XIX, m. 265°, identical (ir spectrum) with authentic XIX. Investigation of S-oxide formation with V and substituted V by H2O2 gave the following results [starting compound, solvent, FeCl3 reaction, Rf value (TLC on silica gel G with 3:1 C6H6-MeOH) given]: V, Me2SO, blue (indicative of S-oxide formation), -; 1-Me derivative (XX) of V, MeOH-CHCl3 + Et3N, blue (indicative of S-oxide formation), 0.07; 6-thiotheobromine, DMF, blue (indicative of S-oxide formation), 0.00; 2-imino derivative of XX, no S-oxide detectable, -; 6-thiocaffeine (XXI), no S-oxide detectable, -. 6-Thiotheophylline (200 mg.) and 1 cc. Et3N in 50 cc. CHCl3 and 50 cc. EtOH kept 15 min. at 50° with 1 cc. 30% H2O2, concentrated as rapidly as possible in vacuo at <30° (bath) until crystallization began, and cooled at -20° gave 158 mg. S-oxide hydrate (XXII.H2O), m. 241-5° (decomposition), Rf 0.29 (TLC on silica gel G with 3:1 C6H6-MeOH); the stability of XXII was attributed to intramol. H bridge formation. XXI (500 mg.) in 15 cc. AcOH heated with 3 cc. 30% H2O2 at 50° (transient deep yellow color formed, but no S-oxide was detectable with FeCl3), after 5 min. the solution diluted with 150 cc. H2O, excess H2O2 destroyed with MnO2, and the solution filtered, concentrated, neutralized with aqueous NH3, and extracted 3 times with CHCl3 gave, from the exts., caffeine, m. 239° (EtOH). V (300 mg.) in 10 cc. DMF kept 90 min. at 30-5° with 1 cc. 30% H2O2, diluted with H2O, and cooled deposited 130 mg. bis(6-purinyl) disulfide (XXIII), identical (TLC on silica gel G with 2:1 C6H6-EtOH) with authentic XXIII. Ir data were given for some compds.

IT **14156-64-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 14156-64-0 CAPLUS

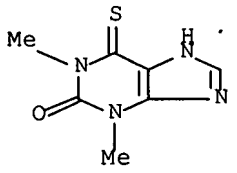
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-sulfinyl- (9CI) (CA INDEX NAME)



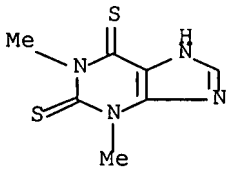
L57 ANSWER 86 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:420841 CAPLUS Full-text
DOCUMENT NUMBER: 65:20841
ORIGINAL REFERENCE NO.: 65:3877f-h,3878a-c
TITLE: Purine derivatives. III. Sulfur-containing theophyllines. I
AUTHOR(S): Merz, K. W.; Stahl, P. H.
CORPORATE SOURCE: Univ. Freiburg/Br., Germany
SOURCE: Beitr. Biochem. Physiol. Naturstoffen, Festschr. (1965) 285-98
DOCUMENT TYPE: Journal
LANGUAGE: German
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB cf. CA 63, 4296b. It is easy to prepare 6-thiotheophylline (I) by heating theophylline with P4S10 in a pyridine base b. 140-60° but 2,6-dithiotheophylline (II) can only be prepared (in very small quantities) from

theophylline by melting it together with P4S10. 2-Thiotheophylline (III) was prepared first. Ethyl cyanoacetate, N,N'-dimethylthiourea, and NaOMe was refluxed 15 hrs. in a mol. ratio of 1.5:1:1.5 to give 34.5% 1,3-dimethyl-4-amino-2-thiouracil (IV), m. 289-90°. IV suspended in H2O and AcOH, or in HCONH2, was cooled in ice and NaNO2 added dropwise to give blue-green 1,3-dimethyl-4-amino-5-nitroso-2-thiouracil (V), m. 218-20°. V was reduced with Na dithionate at 100°, when 2-5 g. IV was used. When 10-30 g. IV was used, Na dithionate was used as starter, but the reduction itself was effected by formic acid. In both cases, 1,3-dimethyl-4,5-diamino-2-thiouracil (VI), m. 240-3°, was formed, and when HCONH2 was still present, 1,3-dimethyl-4-amino-5-formylamino-2- thiouracil (VII), m. 304-5°, was formed immediately. By heating VII for 0.5 hr., III, m. 344-8°, was formed, from which II, m. 267-9°, was prepared with P4S10 in pyridine with 1% H2O. It was not possible to prepare the nitroso compound from the orange 1,3dimethyl-4-amino- 2,6-dithiouracil (VIII), m. 273-5° (prepared from IV with P4S10), or from 1,3-dimethyl-4-amino-6-thiouracil (IX), m. 283-6° because of the lower electronegativity of the S, compound with the original O. By boiling 1,3-dimethyl-4,5-diaminouracil (X) or VI 12 hrs. with P4S10 in pyridine, 1,3-dimethyl-4,5-diamino-6-thiouracil (XI), and 1,3-dimethyl-4,5-diamino-2,6-dithiouracil (XII) were prepared, resp. With formamide the ring was closed and I, m. 311°, and II, were formed. From VI in stoichiometric ratio with HNO2 4,5,6,7-tetrahydro-4,6-dimethyl- 5-thio-7-oxo-v-triazolo[4,5-d]pyrimidine (XIII), m. 229°, was obtained; this was not possible with XI and XII. The S in III and I was substituted by 2H, by boiling the compound with Raney Ni in a dilute NH3 solution, to give 1,2,3,6-tetrahydro-1,3-dimethyl-6-oxopurine (XIV), and 1,2,3,6-tetrahydro-1,3-dimethyl-2-oxopurine (XV), resp., but neither of the S atoms could be substituted in the same way in II. Identification was by thin-layer chromatography on silica gel with 80:12:5 C6H6-EtOHAcOH. In the uv spectra of the compds. a bathochromic shift of the absorption bands with regard to theophylline was observed. This increased in the order: III, I, II. Also the number of maximum increased, and in methanol solution the intensity of the strongest absorption bands increased in the same order. 21 references.

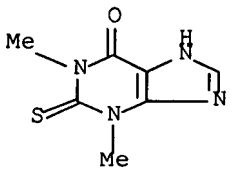
IT **2398-70-1**, Theophylline, 6-thio-
(potassium derivative)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



IT **6501-94-6**, Theophylline, dithio- **6603-63-0**, Theophylline, 2-thio-
(spectrum of)
RN 6501-94-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 6603-63-0 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 87 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:93480 CAPLUS Full-text
DOCUMENT NUMBER: 64:93480
ORIGINAL REFERENCE NO.: 64:17597b-h,17598a-e
TITLE: Syntheses in the purine series. XVII. Syntheses of N,S-purinium betaines
AUTHOR(S): Bredereck, Hellmut; Schellenberg, Peter; Nast, Roland; Heise, Hartmut; Christmann, Otto
CORPORATE SOURCE: Tech. Hochsch., Stuttgart, Germany
SOURCE: Chemische Berichte (1966), 99(3), 944-57
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 64:93480
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB cf. CA 57, 15107e. 7,9-Dimethyl- and 1,7,9-trimethyl-N,S-purinium betaines were prepared by the conversion of OH, SH, or PhCH2S groups in 7,9-dimethyl- and 1,7,9-trimethylpurinium salts, resp., into the SH group and subsequent liberation from the resulting salts. Hypoxanthine (1.5 g.) in 15 g. p-MeC6H4-SO3Me (I) stirred 15 min. at 250° and diluted with 25 cc. BuOH and then 150 cc. Et2O yielded 2.3 g. 6-hydroxy-7,9- dimethylpurinium p-toluenesulfonate (II), m. 255-6° (BuOH). II (3.36 g.) and 80 cc. POCl3 refluxed 2 hrs. and evaporated, treated with 125 cc. absolute EtOH and 7 g. CS(NH2)2 (III), refluxed 2 hrs., cooled, diluted with 400 cc. MeOH, and saturated with dry NH3 yielded 1.14 g. pale yellow IV (R = H) (V), m. 283° (decomposition from 265° with sintering). 2-NH2 derivative (3 g.) of II and 150 cc. POCl3 refluxed 4 hrs., evaporated, treated with 200 cc. absolute EtOH and 10 g. III, refluxed 3.5 hrs., and saturated at 30-5° with dry NH3 yielded 0.375 g. IV (R = NH2) (VI), m. 312° (decomposition) with sintering from 295°. 2-MeS derivative (1.91 g.) of II and 60 cc. POCl3, 60 cc. EtOH, and 5 g. III yielded similarly 0.81 g. IV (R = MeS) (VII), m. 277° (decomposition) with sintering from 265°. 7,9-Dimethylxanthinium p-toluenesulfonate (VIII), 125 cc. POCl3, and 0.38 cc. H2O refluxed 3.5 hrs. and then treated with 150 cc. absolute EtOH and 10 g. III followed by NH3 gave 1.32 g. pale yellow IX (R = H) (X), m. 300°

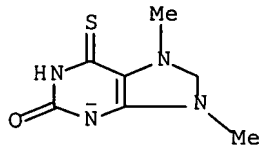
(decomposition) with sintering from 285°. 1-Me derivative (3.66 g.) of VIII gave similarly 0.64 g. XI (R = Me) (XII), m. 248° (MeOH). 2-Amino-6-mercaptopurine (0.5 g.) and 5 g. I stirred 10 min. at 117°, diluted with an equal volume EtOH, and treated dropwise with dry Et2O gave 0.86 g. VII, m. 281°. VII (2.5 g.) added in portions with stirring to Cl in absolute MeOH gave 0.75 g. 2-amino-6-chloro-7,9-dimethylpurinium chloride (XIII), m. 293° (EtOH); picrate, m. 209° (EtOH). XIII (0.5 g.), 80 cc. absolute EtOH, and 0.5 g. III refluxed 4 hrs. yielded 0.32 g. pale yellow-green 6-SH analog (XIV) of XIII, m. 275°. XIV in MeOH treated with dry NH3 gave VI. 6-Hydroxy-2-thioxodihydropurine (1.68 g.) in 0.4 g. NaOH in 50 cc. H2O treated dropwise with stirring at room temperature during 1 hr. with 1.61 g. PhCH2-Cl in 20 cc. MeOH and stirred 4 hrs. yielded 1.6 g. 6-hydroxy-2-benzylthiopurine (XV), m. 262-3° (absolute EtOH). XV (0.5 g.) and 5 g. I yielded 0.69 g. 6-hydroxy-2-benzylthio-7,9-dimethylpurinium p-toluenesulfonate (XVI), m. 240° (EtOH). 2,6- Dithioxotetrahydropurine (2.3 g.) in 250 cc. H2O and 1.6 g. NaOH treated dropwise during 2 hrs. with 4.6 g. PhCH2Br in 20 cc. MeOH and stirred 5 hrs. yielded 3.1 g. 2,6-bis(benzylthio)purine (XVII), m. 196° (absolute EtOH). XVII (2.5 g.) and 20 g. I stirred 10 min. at 170° yielded 2.02 g. 2,6-bis(benzylthio)7,9-dimethylpurinium p-toluenesulfonate (XVIII), m. 170° (absolute EtOH). 2-Benzylthio-6-thioxo-1- methyldihydropurine (3 g.) and 20 g. I stirred 1 hr. at 150°, cooled, and diluted with 20 cc. absolute EtOH and 500 cc. Et2O, and the oily precipitate treated in 500 cc. boiling H2O with 10 cc. 65% HClO4 yielded 2.4 g. 2-benzylthio-6-thioxo-1,7,9-trimethyldihydropurinium perchlorate (XIX), m. 177° (absolute EtOH). 2-Amino-6-benzythiopurine (0.5 g.) and 5 g. I gave similarly after treatment of the product with 65% HClO4 0.56 g. 2-amino-6-benzylthio-7,9-dimethylpurinium perchlorate (XX), m. 226° (EtOH). XVI (0.5 g.), 2 g. AlBr3, and 60 cc. dry MePh stirred 6 hrs. at 80° gave 0.16 g. XI (R = H) (XXI), m. 297° (H2O). XVIII (1 g.), 4.0 g. AlBr3, and 100 cc. dry MePh gave similarly 0.34 g. (crude) pale yellow XXII (R = H) (XXIII), m. 283° (decomposition) (H2O). XIX (1 g.), 5 g. AlBr3, and 150 cc. dry MePh yielded similarly 0.245 g. (crude) yellow XXII (R = Me) (XXIV), m. 255° (decomposition). XX (0.5 g.), 2 g. AlBr3, and 60 cc. dry MePh gave 0.24 g. pale yellow 2-amino-6-mercapto-7,9- dimethylpurinium bromide, m. 270° (EtOH); a 0.5-g. portion in 25 cc. MeOH treated with dry NH3 gave 0.31 g. VI, m. 312°. 6-Oxo-2-thioxo-3-methyltetrahydropurine (4.0 g.) in 250 cc. H2O and 2.0 g. NaOH with 4.1 g. PhCH2Br yielded 4.6 g. 2-benzylthio-6-oxo-3-methyldihydropurine (XXV), m. 218° (absolute EtOH). XXV (1.0 g.) and 5.0 g. I stirred 45 min. at 150°, and the oily product treated in 100 cc. BuOH with 3 cc. 65% HClO4 and then 200 cc. Et2O yielded 0.56 g. 2-benzylthio-6-oxo-3,7,9-trimethyldihydropurinium perchlorate (XXVI), m. 202° (absolute EtOH). XXVI (1.0 g.), 5.0 g. AlBr3, and 150 cc. dry MePh yielded 0.45 g. (crude) 6-oxo-2-thioxo-3,7-dimethyltetrahydropurine, m. 308° (with sintering from 290°) (H2O). V (0.200 g.) added in portions to 1 cc. 30% H2O2, and the sirupy product in 20 cc. MeOH treated successively with 0.5 cc. 30% H2O2 and dry NH3 gave 0.115 g. 6-hydroxy-7,9-dimethylpurinium betaine (XXVII). Hypoxanthine (1.5 g.) in 15.0 g. I stirred 15 min. at 150° gave 2.3 g. 6-hydroxy-7,9- dimethylpurinium p-toluenesulfonate (XXVIII), m. 255-6° (BuOH). XXVIII (1.5 g.) in 150 cc. hot MeOH treated at room temperature with dry NH3 gave 0.5 g. XXVII, m. 309°. XXVII (about 100 mg.) in 10-20 cc. MeOH treated with 5-6 drops 65% HClO4 gave the perchlorate analog of XXVIII, m. 171° with sintering from 130° (BuOH). X.H2O (0.400 g.) added in portions at 30° to 2 cc. 30% H2O2 and treated after 2 hrs. with dry NH3 yielded 0.175 g. 7,9-dimethylxanthinium betaine (XXIX) (perchlorate, m. 281°), which was also obtained similarly from VII, XXI, and XXIII. 2-Hydroxy-6-thioxo1-methyldihydropurine (3.64 g.) and 6.0 g. I in 25 cc. AcNMe2 heated 15 min. at 145° gave 4.13 g. (crude) 2-hydroxy-6-thioxo-1,7,9-trimethyldihydropurinium p-toluenesulfonate; a 3.00-g. portion in 150 cc. MeOH treated at room temperature with concentrated NH4OH yielded 0.85 g. 2-hydroxy-6-thioxo-1,7,9- trimethyldihydropurinium betaine (XXX), m. 355-7° (decomposition) (H2O). The oxidation of XXX with H2O2 gave 1,7,9-trimethylxanthinium betaine (XXXa) which was also obtained from XII and XXIV.

VI oxidized similarly gave 2-amino-6-hydroxy-7,9-dimethylpurinium betaine (XXXI). The Rf values were determined with 2:1 BuOH-5N AcOH (A), 2:1 PrOH-H2O (B), 5% aqueous NH4Cl (C), and 4% aqueous Na citrate (D), and the pKa, values in H2O at 20° were measured potentiometrically or spectroscopically for the compds. listed in the table. The uv spectra of X, XII, XXI, XXIII, XXIV,XXX are recorded.Compound, A, B, C, D, pKa; V, 0.40, 0.60, 0.81, 0.80, 5.56 ± 0.04; VI, 0.41, 0.51, 0.66, 0.71, 6.28 ± 0.03; VII, 0.62, 0.75, 0.74, 0.66, 4.74 ± 0.08; X, 0.32, 0.50, 0.70, 0.65, 1.9 ± 0.2; XXX, 0.58, 0.72, 0.69, 0.66, 2.1 ± 0.2; XXI, 0.25, 0.41, 0.77, 0.73, 1.85 ± 0.2; XII, 0.42, 0.63, 0.79, 0.76, 1.95 ± 0.2; XXIII, 0.38, 0.57, 0.63, 0.58, 0.83 ± 0.13; XXIV, 0.57, 0.75, 0.57, 0.55, 0.71 ± 0.04; XXVII, 0.28, 0.50, 0.58, 0.87, --; XXXI, 0.30, 0.46, 0.81, 0.84, --; XXIX, 0.21, 0.38, 0.85, 0.76, --; XXXa, 0.40, 0.58, 0.90, 0.84, --; .

IT **5752-14-7P**, Purinium compounds, 1,6-dihydro-2-hydroxy-7,9-dimethyl-6-thioxo-, hydroxide, inner salt **5752-18-1P**, Purinium, 1,6-dihydro-2-hydroxy-1,7,9-trimethyl-6-thioxo-, hydroxide, inner salt **5752-62-5P**, Purinium, 1,6-dihydro-2-mercapto-7,9-dimethyl-6-oxo-, hydroxide, inner salt **5752-63-6P**, Purinium, 1,6-dihydro-2-mercapto-7,9-dimethyl-6-thioxo-, hydroxide, inner salt **5752-64-7P**, Purinium, 1,6-dihydro-2-mercapto-1,7,9-trimethyl-6-thioxo-, hydroxide, inner salt **5992-44-9P**, Purinium, 1,6-dihydro-2-mercapto-1,7,9-trimethyl-6-oxo-, hydroxide, inner salt
RL: PREP (Preparation)
(preparation of)

RN 5752-14-7 CAPLUS

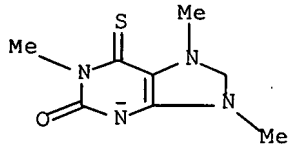
CN Purinium, 1,6-dihydro-2-hydroxy-7,9-dimethyl-6-thioxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 5752-18-1 CAPLUS

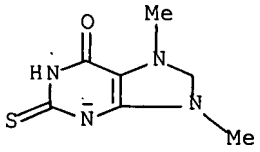
CN Purinium, 1,6-dihydro-2-hydroxy-1,7,9-trimethyl-6-thioxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



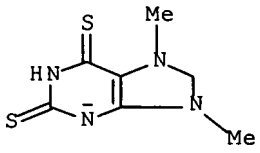
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 5752-62-5 CAPLUS

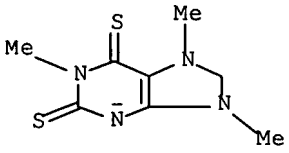
CN Purinium, 1,6-dihydro-2-mercapto-7,9-dimethyl-6-oxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



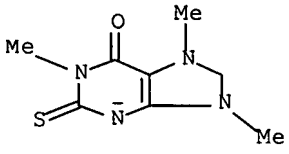
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 5752-63-6 CAPLUS
CN Purinium, 1,6-dihydro-2-mercapto-7,9-dimethyl-6-thioxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 5752-64-7 CAPLUS
CN Purinium, 1,6-dihydro-2-mercapto-1,7,9-trimethyl-6-thioxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



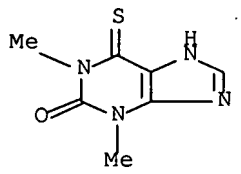
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 5992-44-9 CAPLUS
CN Purinium, 1,6-dihydro-2-mercapto-1,7,9-trimethyl-6-oxo-, hydroxide, inner salt (8CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

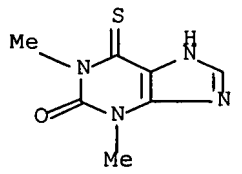
L57 ANSWER 88 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1966:11492 CAPLUS Full-text
DOCUMENT NUMBER: 64:11492
ORIGINAL REFERENCE NO.: 64:2087a-d
TITLE: Demethylation of 3-methyl-6-methylthiopurines with hydrogen sulfide

AUTHOR(S): Neiman, Z.; Bergmann, F.
CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem
SOURCE: Israel J. Chem. (1965), 3(3), 85-9
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB The title compds., with the quinonoid form of the imidazole ring, readily undergo thiohydrolysis in aqueous solution (I, R = H), (II, R = H), (VII), , (VIII); (III, R = Me), (IV, R = Me), , , , ; (V, R = Ph), (VI, R = Ph), , , , Thus, H2S bubbled during 20 min. at room temperature through a suspension of I in 25% NH4OH and the solution evaporated to dryness in vacuo gives 70% II. Similarly, III gives 60% IV, decomposed 300° (AcOH); V in Me2NCHO containing 0.1 volume N NaOH gives VI, decomposed 280-5° (dilute AcOH); and VII gives 80% VIII. 6-Methylthiopurine (non-quinonoid imidazole ring) is unchanged under the same conditions. A mixture of 22 g. 8-phenylhypoxanthine, 100 g. P2S5, and 500 ml. dry β-picoline was stirred and refluxed 4 hrs., the solvent removed in vacuo, the residue treated 1 hr. with 200 ml. H2O at 70°, the insoluble material triturated with 2N NaOH, and the mixture filtered through Celite. The solution was decolorized with C, acidified with AcOH, the precipitate dissolved in 5% Na2CO3, the solution heated with C, filtered, and cooled. The Na salt which separated was dissolved in hot H2O and hot saturated aqueous NH4Cl added to give 80% yellow needles of 6-mercapto-8-phenylpurine (IX), decomposed 300°. A solution of 39 g. IX in 600 ml. Me2NCHO containing 75 ml. MeI was refluxed 2 hrs., 40 ml. MeI added, reflux continued 2 hrs., and the mixture cooled. The yellow precipitate was dissolved in H2O and the pH adjusted to 10 with 2N NaOH to yield 48% V, m. 196-8° (iso-PrOH). Similarly, 6-mercapto-8-methylpurine gave 47% III, m. 195° (MeCN). A solution of 2.5 g. 6-thiotheophylline (VIII) in 15 ml. N NaOH stirred 4 hrs. at room temperature with 2.5 ml. MeI, neutralized with AcOH, evaporated to dryness in vacuo, and the residue extracted with iso-PrOH gave 22% VII, m. 189-91° (iso-PrOH). Uv and chromatographic data are given.
IT **2398-70-1**, Theophylline, 6-thio-
(spectrum of)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 89 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:400859 CAPLUS Full-text
DOCUMENT NUMBER: 63:859
ORIGINAL REFERENCE NO.: 63:129g-h
TITLE: Mass spectrum of thiotheophylline
AUTHOR(S): Chaigneau, Marcel; Valdener, Georges; Seyden-Penne, Jacqueline
CORPORATE SOURCE: C.N.R.S., Paris
SOURCE: Compt. Rend. (1965), 260(14 (Groupe 8)), 3965-8

DOCUMENT TYPE: Journal
LANGUAGE: French
ED Entered STN: 22 Apr 2001
AB The mass spectrum has a relatively very intense mol. peak, and several other peaks which are explained by fragmentation and rearrangement processes. The analogy with the fragmentation mode of theophylline is striking.
IT **2398-70-1**, Theophylline, 6-thio-
(mass spectrum of)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)

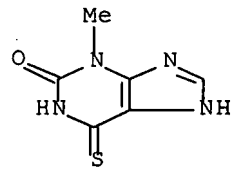


L57 ANSWER 90 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:425465 CAPLUS Full-text
DOCUMENT NUMBER: 61:25465
ORIGINAL REFERENCE NO.: 61:4377g-h,4378a
TITLE: Purine derivatives
INVENTOR(S): Hitchings, George H.; Elion, Gertrude B.
PATENT ASSIGNEE(S): Burroughs Wellcome & Co. (U.S.A.) Inc.
SOURCE: 2 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3135754		19640602	US 1962-215774	19620809 <--
PRIORITY APPLN. INFO.:			US	19620809 <--

ED Entered STN: 22 Apr 2001
AB Continuation-in-part of U.S. 3,056,785 (CA 58, 5701e). These new compds., useful when used in combination with p-aminobenzoic acid antagonists, strongly inhibited Proteus vulgaris (strain 49210 I), and were active against transplantable rodent tumors such as Adenocarcinoma 755. A solution of 25 g. 6-iodopurine (I) and 16.8 g. 6-mercaptopurine hydrate in 100 ml. 2N NaOH steam bath heated 24 hrs., was cooled and neutralized with AcOH. The yellow precipitate of 22 g. 6,6-dipurinyl sulfide dihydrate (II) was collected, washed with H2O, and dried in vacuo. A mixture of 2.5 g. I, 1.12 g. 4-mercaptopyrimidine, and 10 ml. 2N NaOH yielded 6-(4- pyrimidinyl)thiopurine (III), m. 184-5° (decomposition). A mixture of 7.3 g. 6-thioguanine, 10 g. I, and 60 ml. 2N NaOH yielded 6-(2-amino-6- purinyl)thiopurine (IV), not melting above 325°. A mixture of 10 g. I, 5.12 g. 4-thiouracil, and 60 ml. 2N NaOH yielded 6-(2-hydroxy-4- pyrimidinyl)thiopurine (V). The ultraviolet absorption spectrum showed maximum λ 275 and 308 mμ at pH 1, and 285 and 312 mμ at pH 11 for II; at 273 and 300 mμ at pH 1, and 280 and 305 mμ at pH 11 for III; at 270, 302, and 330 mμ at pH 1, and 287 and 328 mμ at pH 11 for IV; and at 320 mμ at pH 1, and 310 mμ at pH 11 for V.
IT **33285-76-6P**, Purin-2(3H)-one, 6-mercapto-3-methyl-

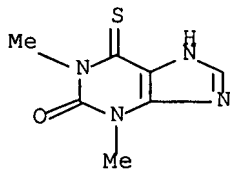
RL: PREP (Preparation)
(preparation of)
RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



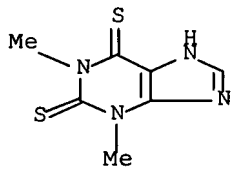
L57 ANSWER 91 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:425464 CAPLUS Full-text
DOCUMENT NUMBER: 61:25464
ORIGINAL REFERENCE NO.: 61:4377e-g
TITLE: Alkylthiopurines
INVENTOR(S): Hitchings, George H.; Elion, Gertrude B.
PATENT ASSIGNEE(S): Burroughs Wellcome & Co. (U.S.A.) Inc.
SOURCE: 2 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3135753		19640602	US 1961-108986	19610510 <--
PRIORITY APPLN. INFO.:			US	19610510 <--

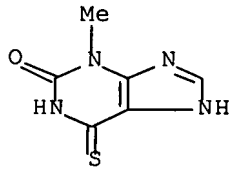
ED Entered STN: 22 Apr 2001
AB The title compds. possess a much improved coronary flow index, 4 and 5, compared to 1 for aminophylline, and are useful in relieving the symptoms angina pectoris. A mixture of 4.3 g. 3-methylhypoxanthine, 12 g. powdered P2S5, and 100 ml. dry pyridine (I) was refluxed 2.5 hrs., I removed in vacuo, and the solid residue heated with 200 ml. H2O for 20 min. to give 3.25 g. 3-methyl-6-purinethione (II), m. of 322-3° (decomposition). A mixture of 10 g. 1,3-dimethylxanthine (III), 50 g. powdered P2S5, and 150 ml. Tetralin heated 5 hrs. at 190° yielded 5.2 g. 2,6- dithiotheophylline, m. 252-4° (decomposition). A mixture of 5 g. III, 15 g. P2S5, and 150 ml. I refluxed 2 hrs. yielded 3.5 g. crude 6-thiotheophylline, m. 315-17° (decomposition). A mixture of 1 g. 3-methylxanthine, 5 g. P2S5, and 50 ml. I refluxed 3 hrs. yielded 0.7 g. 3-methyl-2-oxo-6-mercaptopurine, decompose 320°. A mixture of 5.6 g. 3-methyl-2-thioxanthine, 20 g. P2S5, and 250 ml. I refluxed yielded 3.2 g. 3-methyl-2,6-dithioxanthine, m. >340°. The ultraviolet absorption spectra of these compds. were given. Cf. CA 50, 1933c.
IT **2398-70-1P**, Theophylline, 6-thio- **6501-94-6P**, Theophylline, dithio- **33285-76-6P**, Purin-2(3H)-one, 6-mercapto-3-methyl- **33285-77-7P**, Xanthine, 3-methyl-2,6-dithio-
RL: PREP (Preparation)
(preparation of)
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



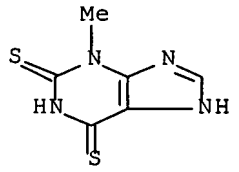
RN 6501-94-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)

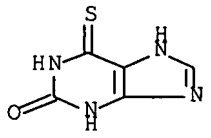


RN 33285-77-7 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)

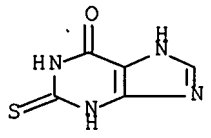


L57 ANSWER 92 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:84708 CAPLUS Full-text
DOCUMENT NUMBER: 60:84708
ORIGINAL REFERENCE NO.: 60:14874c-e
TITLE: Action of 8-azaguanine and 8-azaxanthine on Pseudomonas aeruginosa
AUTHOR(S): Bergmann, F.; Ungar-Waron, Hanna; Kwietny-Govrin,

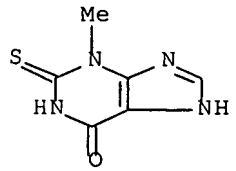
Hanna
CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School
SOURCE: (**1964**), 91(2), 270-6
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB 8-Azaguanine does not inhibit the growth of P. aeruginosa, but undergoes slow deamination. 8-Azaxanthine arrests the growth of this species temporarily. This growth retardation is abolished by hypoxanthine, xanthine, and a number of unnatural purines. During growth inhibition by azaxanthine, the xanthine oxidase-like activity of the bacterial cells is enhanced. Much larger increments of enzymic activity are obtained by the addition of hypoxanthine, xanthine, or certain unnatural purines, which all contain an unsubstituted imidazole ring. During growth inhibition by 8-azaxanthine, the urate oxidase-like activity of the bacteria is strongly depressed. On the other hand, the addition of hypoxanthine or xanthine to the culture medium produces a huge increase in the enzymic activity of the normal strain. After the 1st exposure to 8-azaxanthine a resistant strain emerges. This strain shows normal xanthine oxidase and urate oxidase activities, even when growing in the presence of the antimetabolite. Benzimidazole and benzotriazole are weak growth inhibitors. They depress xanthine oxidase activity of the bacterial cells, but leave their urate oxidase activity unaffected.
IT **2002-59-7**, Xanthine, 6-thio- **2487-40-3**, Xanthine, 2-thio- **28139-02-8**, Xanthine, 3-methyl-2-thio-
(effect on Pseudomonas aeruginosa response to 8-azaxanthine)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



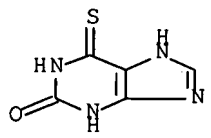
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



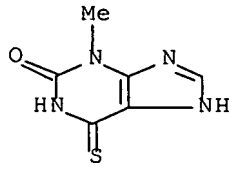
RN 28139-02-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



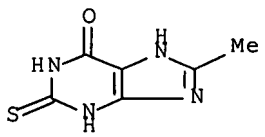
L57 ANSWER 93 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:60225 CAPLUS Full-text
DOCUMENT NUMBER: 60:60225
ORIGINAL REFERENCE NO.: 60:10497a-b
TITLE: Kinetic studies on the methylation of thiopurines
AUTHOR(S): Bergmann, F.; Kleiner, M.
CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem
SOURCE: Israel J. Chem. (1963), 1, 477-82
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB Reaction of 6-mercaptopurine (I) with MeI in HCONMe2 was followed by paper chromatography and ultraviolet spectra; in a 2 step process, viz., alkylation at the S atom, followed by alkylation at N3, it gave 3-methyl-6-methylthiopurine. 6-Thioxanthine (II) underwent a similar 2 step methylation. Comparison of kinetics of the 2 systems (i.e. with I and II) and the exceedingly fast rate of S-methylation of 3-methyl-6-purinethione (III) showed that I reacted through a tautomeric form having a quinonoid structure in the pyrimidine ring. A similar fixed quinonoid structure in III explained its fast methylation. The S-Me group had no marked influence on alkylation at N3.
IT **2002-59-7**, Xanthine, 6-thio- **33285-76-6**, Xanthine, 3-methyl-6-thio-
(methylation of)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



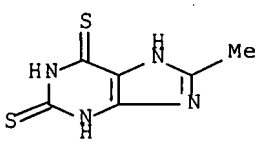
RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



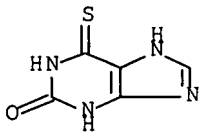
L57 ANSWER 94 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:9768 CAPLUS Full-text
DOCUMENT NUMBER: 60:9768
ORIGINAL REFERENCE NO.: 60:1748a-d
TITLE: Direct thiation of pyrimidinol derivatives
AUTHOR(S): Ueda, Takeo; Tsuji, Tadakazu; Momona, Hiroko
CORPORATE SOURCE: Keio-Gijuku Univ., Tokyo
SOURCE: Chemical & Pharmaceutical Bulletin (1963), 11(7), 912-17
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 60:9768
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB 2-Methyl-6-amino-4-pyrimidinethiol, yellow, m. 298° (decomposition); 6-amino-2,4-pyrimidinedithiol, yellow,m. 309° (decomposition); and 2-methyl-5,6-diamino-4-pyrimidinethiol, brownish-yellow, m. 28,5° (decomposition) were prepared in 40 to 50% yield by refluxing 0.005 mol of the appropriate amino-4-pyrimidinol and 0.0125 mol P2S5 in 20 mL. Et3N or 3-picoline for 1 to 15 h. After concentration in vacuo the residue was poured into H2O, made basic with NaOH, filtered hot, neutralized with AcOH, chilled, and the precipitated product recrystd. from H2O. The appropriate 5-acylamino-6-amino-4-pyrimidinols (I) refluxed 8 h. with P2S5 in pyridine, the solvent removed in vacuo, the residue dissolved in H2O, kept 12 h., warmed 1 h. on a water bath, made basic, and chilled, gave II (R1, R2, R3, m.p., and % yield given): NH2, NH2, Me, 248-50°, 81.1; Me, NH2, Me, 192-4°, 81.5. Adjusting the filtrate to pH 5.6 gave III (R1, R2, R3, m.p., % yield given): Me, SH, Me, >300°, 12.2; SH, OH, Me, >300°, 89; SH, SH, Me, >300°, 86.9; Me, SH, H, -, -; Me, SH, OH, (from I, R3 = OEt), >300°, -. Similarly, III (R1 = NH2, R2 = OH, R3 = Et), reacts with P2S5 in pyridine to form III (R1 = NH2, R2 = SH, R3 = Et), orange-yellow, m. >300°. None of these compds. shows significant activity against poliomyelitis virus.
IT **91184-09-7P**, Xanthine, 8-methyl-2-thio- **91184-18-8P**, Xanthine, 8-methyl-2,6-dithio-
RL: PREP (Preparation)
(preparation of)
RN 91184-09-7 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-2-thioxo- (9CI) (CA INDEX NAME)



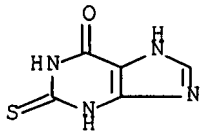
RN 91184-18-8 CAPLUS
CN Xanthine, 8-methyl-2,6-dithio- (7CI) (CA INDEX NAME)



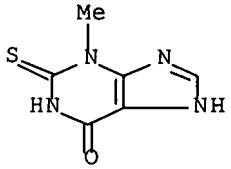
L57 ANSWER 95 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:60954 CAPLUS Full-text
DOCUMENT NUMBER: 58:60954
ORIGINAL REFERENCE NO.: 58:10464a-e
TITLE: Relation of structure to the inhibitory activity of purines against urate oxidases
AUTHOR(S): Bergmann, F.; Kwietny-Govrin, Hanna; Ungar-Waron, Hanna; Kalmus, A.; Tamari, M.
CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem
SOURCE: Biochemical Journal (1963), 86, 567-74
CODEN: BIJOAK; ISSN: 0264-6021
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB cf. ibid. 292. The inhibitory activity of a variety of compds. against urate oxidase has been determined: I50 values in μM were for hypoxanthine 220, 8-hydroxy-purine 110, 2-hydroxypurine 12, 2,8-dihydroxypurine 5.2, xanthine 18, 6,8-dihydroxypurine 66, 6-mercaptopurine 700, 6-thioxanthine 2.7, 2-thioxanthine 190, 8-hydroxy-6-mercaptopurine 70, 6-hydroxy-8-mercaptopurine 500, 6,8-dimercaptopurine 370, 8-hydroxy-2-mercaptopurine 500, 2-hydroxy-8-mercaptopurine 12, 2-thiouric acid 250, 6-thiouric acid 14, 8-thiouric acid 5, 2,6-dithiouric acid 150, 2,8-dithiouric acid 80, 6,8-dithiouric acid 0.4, 6,8-dihydroxy2- methylmercaptopurine 500, 2,6-dihydroxy-8-methylmercaptopurine 38, 2-hydroxy-6-methylmercaptopurine 6, 8-hydroxy-6methylmercaptopurine 32, 2,8-dihydroxy-6-methylmercaptopurine 0.1,3, 8-hydroxy-3-methyl-6- methylmercapto-2-oxopurine 7, 4,5-diamino-6-thiouracil 38, 2,4-dihydroxypteridine 300, 2,4,6trihydroxypteridine 150, 2,4,6,7-tetrahydroxypteridine 500, 8-aza-6-hydroxypurine 47, 8-aza-2-hydroxypurine 1.6, 8-azaxanthine 5.9, 3-methyl-2-thiouric acid 150, 3-methyl-6-thiouric acid 400, 3-methyl-8-thiouric acid 190, 3-methyl-2-thioxanthine 100, 3-methyl-6-thioxanthine 100, 7-methyl-6-thioxanthine 1000. The inhibitory effect was used to measure the affinity of the inhibitors for the enzyme. Of the 3 O atoms of uric acid, that of the 2-carbonyl group possesses the greatest binding power for the active center. Replacement of this O atom by S greatly diminishes the inhibitory activity. Combination of a 2-carbonyl group with S at C-6 enhances inhibitory activity considerably. On certain purine derivs., a 6-methylmercapto substituent is more effective than a 6-thiocarbonyl group. 2,6-Dihydroxy-6methylmercaptopurine is the most potent inhibitor of urate oxidase known so far. Replacement of the imidazole moiety of the purine ring by triazole enhances affinity, whereas introduction of the pyrazine ring, as in pteridines, greatly decreases it. Free imino groups are essential for the attachment of purines to urate oxidase, as N-methylation weakens or abolishes the inhibitory effect. On the other hand, in 2-thiopurines, methylation at N-3 increases the inhibitory power.
IT **2002-59-7**, Xanthine, 6-thio- **2487-40-3**, Xanthine, 2-thio- **28139-02-8**, Xanthine, 3-methyl-2-thio- **33285-76-6**, Xanthine, 3-methyl-6-thio-
(uric oxidase inhibition by)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



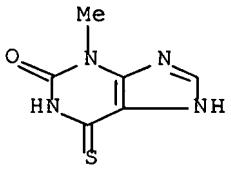
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



RN 28139-02-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)

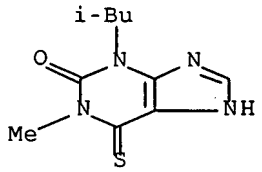


RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 96 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:48836 CAPLUS Full-text
DOCUMENT NUMBER: 58:48836
ORIGINAL REFERENCE NO.: 58:8327a-b
TITLE: Observations concerning the effects of a thioxanthine upon the heart of the intact animal
AUTHOR(S): Maxwell, G. M.; Elliott, R. B.; Kneebone, G. M.

CORPORATE SOURCE: Univ. Adelaide
SOURCE: Australian J. Exp. Biol. Med. Sci. (1962), 40, 335-40
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB An intravenous dose of 1.0 mg. 3-isobutyl-1-methyl-6-thioxanthine/kg. administered to dogs gave statistically significant increases in respiratory rate, respiratory volume, O consumption, CO2 production, and pulse rate. Femoral and pulmonary arterial pressures decreased as did the calculated total peripheral resistance. Coronary blood flow and cardiac metabolic rates for O and CO2 increased. Cardiac efficiency and coronary vascular resistance decreased.
IT **42458-91-3**, Xanthine, 3-isobutyl-1-methyl-6-thio-
(heart response to)
RN 42458-91-3 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)

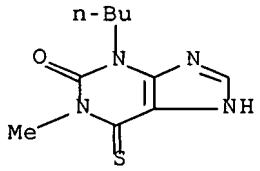


L57 ANSWER 97 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:20789 CAPLUS Full-text
DOCUMENT NUMBER: 58:20789
ORIGINAL REFERENCE NO.: 58:3445a-b
TITLE: 3-Butyl-1-methyl-6-thioxanthine
PATENT ASSIGNEE(S): May & Baker Ltd.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR M188		19610320	FR	19600812 <--
PRIORITY APPLN. INFO.:			FR	19600812 <--

OTHER SOURCE(S): MARPAT 58:20789
ED Entered STN: 22 Apr 2001
AB The title compound can be used in compns. which dilate bronchial tubes. PS5 (56 g.) is added to 33 g. 3-butyl-1-methylxanthine and 500 ml. anhydrous pyridine, the mixture refluxed 8 hrs., cooled, 1000 ml. H2O added carefully, the mixture evaporated in vacuo, the precipitate filtered off, washed with H2O, dissolved in 300 ml. 0.8N NaOH, and the solution acidified with HOAc to give 35 g. 1-methyl-3-butyl-6-thioxanthine, m. 156-8°.
IT **42458-90-2P**, Xanthine, 3-butyl-1-methyl-6-thio-
RL: PREP (Preparation)
(manufacture of)
RN 42458-90-2 CAPLUS
CN 2H-Purin-2-one, 3-butyl-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA

INDEX NAME)

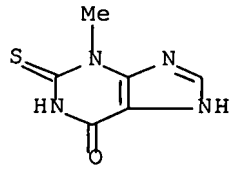


L57 ANSWER 98 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:436343 CAPLUS Full-text
DOCUMENT NUMBER: 57:36343
ORIGINAL REFERENCE NO.: 57:7262i,7263a-e
TITLE: Preparation and properties of 1,2-dihydrophthalazine derivatives
AUTHOR(S): Smith, Richard F.; Otremba, Edward D.
CORPORATE SOURCE: State Univ. Coll., Albany, NY
SOURCE: Journal of Organic Chemistry (1962), 27, 879-82
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:36343
ED Entered STN: 22 Apr 2001
AB cf. CA 53:17143d. Reduction of 2-methyl-and 2-ethylphthalazinium iodide (I, II) with aqueous NaBH4 yielded the corresponding 2-alkyl-1,2-dihydrophthalazines (III, IV). H2O (3 l.) containing 0.3 mole o-HO2CC2H4CHO stirred at 80° with 0.3 mole (N2H4)2.H2SO4 and 1 1.1 .0N NaOH, the green suspension evaporated in vacuo to 200 ml., extracted with C6H6, and the dried (MgSO4) exts. evapd, yielded 50% phthalazine (V), m. 87-90°. Further extraction of the aqueous solution with EtOAc gave 0.9 g. 1(2H)-phthalazinone, m. 183-4°. I, m. 240-3° (decomposition), heated with saturated alc. picric acid (20 ml./g, halide) gave 75% picrate, m. 199-200° (decomposition). II, m. 225-8° (decomposition) (alc.), similarly yielded 93% II picrate, m. 167-9°. V (2 g.) and 4 ml. PhCH2Cl refluxed 3 hrs. in 15 ml. dry MeOH, the cooled mixture diluted with anhydrous Et2O, kept overnight, and the Et2O-washed product dried in vacuo yielded 89% extremely hygroscopic 2-benzylphthalazinium chloride (VI), m. 175-8° (alc.-Et2O); picrate m. 183-4° (MeOH). The powdered quaternary salts added portionwise to 3% aqueous NaBH4 (3:1 salt-hydride), the cooled mixture extracted with Et2O, the extract dried (MgSO4), and the product isolated gave 2-alkyl-1,2-di-hydrophthalazines. Distillation yielded 75% III, b17 129-30°; HCl salt m. 133-5° (decomposition) (alc.); pierate m. 95-8° (decomposition); MeI salt (VII) m. 173-6° (MeOH). III on exposure to air rapidly yielded 2-methyl-1(2H)-phthalazi-none, m. 108-10°. IV HCl salt, m. 142-4° (decomposition) (alc.), converted to the free base, refluxed 6 hrs. with excess MeI in ale., the resultant highly deeompd, tarry product extracted with EtOAc and the extract diluted with Et2O gave IV MeI salt, m. 155-7° (ale.). VI (4.0 g.) reduced with aqueous NaBH4, the oily product refluxed 3 hrs. with 7 ml. MeI in 25 ml. alc., and the mixture cooled gave 1.4 g. VII. Dilution of the filtrate c with Et2O gave 1.4 g. unidentified material, m. 138-42°, recrystd. from alc.-Et2O to give a sample, m. 140-2° (decomposition), melting with evolution of a potent lacrimator. VII (1 g.) in 10 ml. H2O treated with 10 ml. 6N NaOH and the oily product extracted with Et2O gve o-Me2NCH2C4CN; picrate m. 144-5°; MeI salt m. 184-5°; HCl salt m. 226-7° (alc), v 2220 cm.-1, identical with the salt prepd, by stirring 0.05 mole each 0-

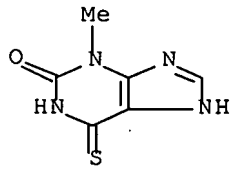
BrCH2C6H4CN, Me2NH.HCl, and anhydrous Na2CO3 2 days at 20° in 50 ml. MeOH, acidifying the coned, solution with dilute HCl, basifying the Et2O-washed aqueous layer, extracting with Et2O, and treating the dried extract with anhydrous HCl.

IT **28139-02-8P**, Xanthine, 3-methyl-2-thio- **33285-76-6P**, Xanthine, 3-methyl-6-thio- **33285-77-7P**, Xanthine, 3-methyl-2,6-dithio- **38695-85-1P**, Xanthine, 1-methyl-6-thio- **91184-08-6P**, Xanthine, 1-methyl-2-thio- **91184-17-7P**, Xanthine, 1-methyl-2,6-dithio-
RL: PREP (Preparation)
(preparation of)

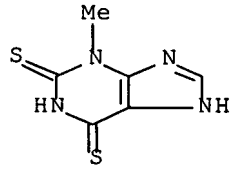
RN 28139-02-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



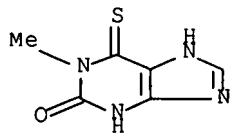
RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



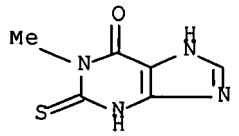
RN 33285-77-7 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



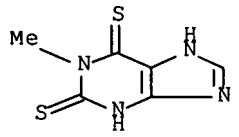
RN 38695-85-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 91184-08-6 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-2-thioxo- (9CI) (CA INDEX NAME)



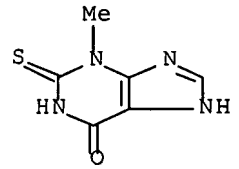
RN 91184-17-7 CAPLUS
CN Xanthine, 1-methyl-2,6-dithio- (7CI) (CA INDEX NAME)



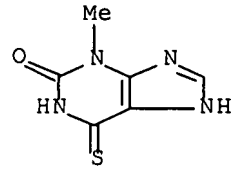
L57 ANSWER 99 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:436342 CAPLUS Full-text
DOCUMENT NUMBER: 57:36342
ORIGINAL REFERENCE NO.: 57:7262h-i
TITLE: Condensed pyrimidine systems. XXII. N-methyl purines
AUTHOR(S): Elion, Gertrude B.
CORPORATE SOURCE: Burroughs Wellcome and Co. Inc., Tuckahoe, NY
SOURCE: Journal of Organic Chemistry (1962), 27, 2478-91
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:36342
ED Entered STN: 22 Apr 2001
AB cf. CA 54, 18531b. A group of 1-and 3-monomethylpurines has been prepared by complete synthesis. Among the new derivs. are 3-methyladenine, 3-methylguanine, and the 1-and 3-methyl derivatives of 6-mercaptopurine. A number of 7- and 9-methyl derivs. have been obtained by direct methylation of 6-chloropurine, conversion to the mercapto derivs., and subsequent separation of the 7- and 9-methylpurine-6-thiols. Several ring openings and rearrangements have been observed in the course of attempts to prepare 1-methyladenine.
IT **28139-02-8P**, Xanthine, 3-methyl-2-thio- **33285-76-6P**, Xanthine, 3-methyl-6-thio- **33285-77-7P**, Xanthine, 3-methyl-2,6-dithio- **38695-85-1P**, Xanthine, 1-methyl-6-thio-

91184-08-6P, Xanthine, 1-methyl-2-thio- **91184-17-7P**, Xanthine, 1-methyl-2,6-dithio-
RL: PREP (Preparation)
(preparation of)

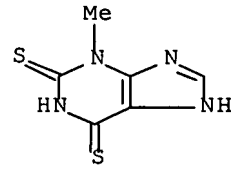
RN 28139-02-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



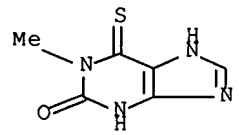
RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



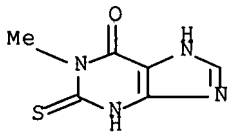
RN 33285-77-7 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



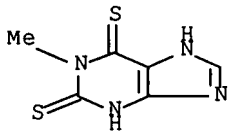
RN 38695-85-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 91184-08-6 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 91184-17-7 CAPLUS
CN Xanthine, 1-methyl-2,6-dithio- (7CI) (CA INDEX NAME)



L57 ANSWER 100 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:429662 CAPLUS Full-text
DOCUMENT NUMBER: 57:29662
ORIGINAL REFERENCE NO.: 57:5924h-i,5925a-i,5926a-b
TITLE: The synthesis of some 6-thioxanthines
AUTHOR(S): Wooldridge, K. R. H.; Slack, R.
CORPORATE SOURCE: May Baker Ltd., Dagenham, UK
SOURCE: Journal of the Chemical Society (**1962**) 1863-28
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:29662
ED Entered STN: 22 Apr 2001
AB A series of 1,3- and 3,7-disubstituted 6-thioxanthines, of interest as broncho and coronary dilators, has been prepared by the selective thionation of the corresponding xanthines with P2S5 in C5H5N. 1,3,7-Trialkyl-6- thioxanthines could not be prepared in this way but were readily obtained front 1,3-dialkyl-6-thioxanthines. Theophylline (50 g.), 100 g. P2S3, and 1. dry C5H5N refluxed 8 hrs. with stirring, cooled, diluted with stirring during 1 hr. with 2 l. H2O, concentrated to about 1/3 volume, cooled, and filtered, and the residue dissolved in 2N NaOH, filtered, and repptd. with dilute HCl yielded 51 g. 1,3-dimethyl-6-thioxanthine (I), pale yellow needles, m. 323-5° (decomposition) (EtOH or H2O). 6-Thiotheobromine (75 g.) with 150 g. P2S5 gave similarly 72 g. 3,7-dimethyl-6-thioxanthine (II), m. 300-1°. (MeNH)2CS (79 g.) added in portions with stirring during 0.5 hr. to 65 g. NCCH2CO2H in 156 g. Ac2O and 200 cc. AcOH at 65°, kept 2 hrs. at 65% evaporated at 69-5° in vacuo, and the gummy residue stirred at 50° with 200 cc. H2O and adjusted to pH 10 with 50% aqueous NaOH gave 65 g. 6-amino-1,3-dimethyl 2-thiouracil (III), prisms, m. 286-8° (EtOH). The crude III suspended in 6000 cc. H2O containing 25.5 g. NaNO2 at 80-90 °, 50 cc. AcOH added during 15 min., and the mixture stirred 15 min. at 80-90° and cooled yielded crude 5-NO derivative (IV) of III, blue-green amorphous solid, m. 215-16° (decomposition). The IV added in 5-g.

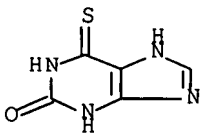
portions to 2.5 l. H2O at 70-80° together with sufficient Na2S2O4 to discharge the color of the IV, cooled, and filtered, the residual 5-NH2 derivative of III, m. 230-4°, added immediately to 500 cc. 2N H2SO4, the resulting sulfate (57 g.) boiled 0.5 hr. with 500 cc. HCONH2, diluted with 250 cc. H2O, and cooled, and the yellow solid dissolved in 300 cc. hot 17% NH4OH, filtered, and acidified to pH 4 with AcOH yielded 47 g. 1,3dimethyl-2-thioxanthine, m. 344-8°. Me2SO4 (25.2 g.) added dropwise in 15 min. with stirring at 40° to 35 g. I and 100 cc. 2N NaOH, kept 0.5 hr. at 40°, cooled, and filtered gave 15 g. 1,3,7-trimethyl-6-thioxanthine (V), pale yellow prisms, m. 246-7°. II (17.5 g.) and 42.5 g. Me2SO4 gave 1 g. V, m. 247-9°. II(10g.)in 125 cc. 0.5N NaOH stirred 2 hrs. at room temperature with 10.7 g. MeI yielded 6.7 g. 1,2,3,4tetrahydro-3,7-dimethyl- 1-methylthiopurine, needles, m. 300-3° (H2O). The appropriate urea was converted by the method of Traube [Ber. 33, 3035(1900)] or of Speer and Raymond (CA 48, 1346h) or of Montgomery (CA 50, 13932b) to the corresponding 1,3-dialkylxanthines (1- and 3-alkyl group and m.p. given): Me, MeO(CH2)3, 166-8°; Me, furfuryl, 255-8°; Et, iso-Bu, 195-7°; Pr, iso-Bu, 189-92°; Bu, Me, 207-10°. Similarly were prepared 3-isobutylxanthine (VI), m. 299-301°, and the 7-Me derivative of VII, m. 239-41°. P2S5 (600 g.) and 482 g. 3-isobutyl-1-methylxanthine in 4.2 l. dry C5H5N, refluxed 9 hrs. with stirring, cooled to about 40°, diluted carefully with H2O, concentrated to about 2.5 1., diluted with 3.5 l. H2O, and filtered, and the residue dissolved in 2.5 l. warm N NaOH, filtered, and acidified with concentrated HCl to pH 4 pp.d. 426 g. 3-isobutyl-1-methyl-6-thioxanthine (VII), yellow prisms, m. 170-2° (EtOH). Similarly were prepared the following 1,3-disubstituted-6-thioxanthines (1- and 3-substituent, m.p., and % yield given): Me, Me (VIII), 3235°, 94; Me, Et, 235-7°, 79; Me, Pr, 164-7°, 63; Me, Bu, 156-8°, 73; Me, Am, 169-70°, 50; Me, C6H13, 167-74°, 78; Me, iso-Am, 156-60°, 50; Me, MeO(CH2)3, 150-2°, 50; Me, CH2:CHCH2, 152-6°, 81; Me, CH:CMeCH2, 195-8°, 47; Me, PhCH2, 213-15°, 84; Me, Ph(CH2)2, 198-9°, 63; Me, furfuryl, 184-6°, 15; Et, Me, 235-9°, 76; Et, Et, 2568°, 72; Et, Bu, 175-8°, 74; Et, iso-Bu, 180-3°, 39; Et, CH2:CHCH2, 210-12°, 49; Pr, Pr, 212-15°, 89; Bu, Me, 295-8°, 84; Bu, Bu, 183-6°, 72. Similarly were prepared the following 8-substituted VIII (substituent, m.p., and % yield given): Me, 294-5°, 75; Et, 218-19°, 76; SH, 240° (decomposition), 83. I (42 g.) and 8.6 g. NaOH in 150 cc. H2O stirred 0.5 hr. at room temperature, cooled, and filtered, and the dried Na salt (44 g.) of I dissolved in 200 cc. HCONMe2, treated with stirring during 15 min. at room temperature with 18.6 g. AcCH2Cl, stirred 0.5 hr., diluted with 300 cc. iced H2O, and filtered gave 21.3 g. 7-AcCH2 derivative (IX) of I, yellow needles, m. 208-10°. IX (21 g.), 269 g. paraformaldehyde, 11.9 g. piperidine-HCl, 1.6 cc. Et2O.BF3, and 200 cc. dry dioxane stirred 7 hrs. at 100° and filtered gave 23.0 g. 1,3-dimethyl-7(2-oxo-4-piperidinobutyl)-6-thioxanthine-HCl, yellow-brown prisms, m. 197-200°. In the same manner as VII were prepared the following 1,3,7-trisubstituted-6-thioxanthines (1-, 3-, and 7-substituents and m.p. given): Me, Me, Et, 22830°; Me, Me, Et2N(CH2)2, 52-4°; Me, iso-Bu, Et2N(CH2)2 |isolated as the (-)-di(p-toluoyl) D-tartrate], 120° (decomposition); Me, iso-Bu, AcCH2, 170-4°; Bu, Me, Me, 118-19°. in the same manner were prepared the following 3,7-dialkyl-6thioxanthines (3- and 7-substituents and m.p. given): Me, Me, 300-1°; Bu, Me, 200-3°; iso-Bu, Me, 228-30°. Also prepared was 3-methyl-6-thioxanthine, m. 269-74°. Choline chloride (3.4 g.) in 900 cc. hot iso-PrOH treated with stirring with 150 g. 85% KOH in 600 cc. absolute MeOH, cooled to 0°, filtered, treated with 500 g. VII, warmed a few min., and evaporated in vacuo, the residual sirup dissolved in 1 l. hot isoPrOH, treated with C, filtered, diluted with 1 l. dry Et2O, and cooled, and the precipitated filtered off gave 548 g. choline salt of VII, pale yellow prisms, m. 145-9°; their mother liquor evaporated, and the sirupy residue dissolved in H2O and acidified to pH 4 with HCl gave 8 g. VII. Similarly were prepared the choline salts of the following 1,3-disubstituted-6-thioxan-thines (1- and 3-substituents, m.p. and % yield given): Me, Me (X), 145-7°, 47; Me, Et, 157-9°, 72; Me, Pr, 145-50°, 72; Me, Bu, 133-5°, 88; Me, Am, 150-3°, 93; Me, C6H13, 55-7°, 94; Me, iso-Bu, 148.5-

9.5°, 92; Me, iso-Am, 125-8°, 90; Me, CH2:CHCH2, 172-5°, 73; Me, CH2:CMeCH2, 145-51°, 80; Me, PhCH2, 166-71°, 80; Me, Ph(CH2)2, 173-5°, 80; Et, Me, 157-8°, 70; Et, Et, 142-7°, 92; Et, Bu, 115-18°, 79; Pr, Pr, 114-18°, 57; Bu, Me, 105-9°, 62. Also prepared were 8-Me derivative of X, 175-6°, 65, and the 8-SH derivative of X, 209 11°, 70. The ultraviolet absorption maximum of a number of thioxanthines are tabulated.

IT **2002-59-7**, Xanthine, 6-thio-
(derivs.)

RN 2002-59-7 CAPLUS

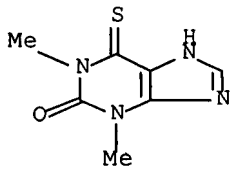
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



IT **2398-70-1P**, Theophylline, 6-thio- **6603-63-0P**, Theophylline, 2-thio- **40915-18-2P**, Xanthine, 1,3-dibutyl-6-thio- **42458-87-7P**, Xanthine, 3-ethyl-1-methyl-6-thio- **42458-88-8P**, Xanthine, 1-methyl-3-propyl-6-thio- **42458-90-2P**, Xanthine, 3-butyl-1-methyl-6-thio- **42458-91-3P**, Xanthine, 3-isobutyl-1-methyl-6-thio- **42458-92-4P**, Xanthine, 1-methyl-3-(2-methylallyl)-6-thio- **42458-93-5P**, Xanthine, 1-methyl-3-pentyl-6-thio- **42458-94-6P**, Xanthine, 3-(3-methoxypropyl)-1-methyl-6-thio- **42458-95-7P**, Xanthine, 3-isopentyl-1-methyl-6-thio- **42458-96-8P**, Xanthine, 3-hexyl-1-methyl-6-thio- **42458-97-9P**, Xanthine, 3-benzyl-1-methyl-6-thio- **42458-98-0P**, Xanthine, 1-methyl-3-phenethyl-6-thio- **42458-99-1P**, Xanthine, 3-furfuryl-1-methyl-6-thio- **42459-00-7P**, Xanthine, 1-ethyl-3-methyl-6-thio- **42459-01-8P**, Xanthine, 1,3-diethyl-6-thio- **42459-02-9P**, Xanthine, 3-allyl-1-ethyl-6-thio- **42459-03-0P**, Xanthine, 3-butyl-1-ethyl-6-thio- **42459-04-1P**, Xanthine, 1-ethyl-3-isobutyl-6-thio- **42459-06-3P**, Xanthine, 1,3-dipropyl-6-thio- **42459-07-4P**, Xanthine, 1-butyl-3-methyl-6-thio- **42459-09-6P**, Xanthine, 1,3,8-trimethyl-6-thio- **42459-10-9P**, Theophylline, 8-ethyl-6-thio- **90230-11-8P**, Choline, compound with 6-thiotheophylline **93263-24-2P**, Xanthine, 3-isobutyl-6-thio- **96536-20-8P**, Choline, compound with 3-ethyl-1-methyl-6-thioxanthine **96536-21-9P**, Choline, compound with 1,3,8-trimethyl-6-thioxanthine **96652-89-0P**, Choline, compound with 1-ethyl-3-methyl-6-thioxanthine **96986-49-1P**, Xanthine, 1,3-diethyl-6-thio-, compound with choline **97212-72-1P**, Choline, compound with 1-methyl-3-propyl-6-thioxanthine **97282-72-9P**, Choline, compound with 3-allyl-1-methyl-6-thioxanthine **97406-00-3P**, Choline, compound with 3-isobutyl-1-methyl-6-thioxanthine **97406-02-5P**, Choline, compound with 3-butyl-1-methyl-6-thioxanthine **97439-87-7P**, Xanthine, 1-butyl-3-methyl-6-thio-, compound with choline **97616-67-6P**, Choline, compound with 3-butyl-1-ethyl-6-thioxanthine **97767-38-9P**, Xanthine, 1-methyl-3-pentyl-6-thio-, compound with choline **97767-40-3P**, Choline, compound with 1,3-dipropyl-6-thioxanthine **97783-97-6P**, Choline, compound with 3-isopentyl-1-methyl-6-thioxanthine **98174-21-1P**, Choline, compound with 3-hexyl-1-methyl-6-thioxanthine **98801-33-3P**, Choline, compound with 3-benzyl-1-methyl-6-thioxanthine **99688-81-0P**,

Choline, compound with 1-methyl-3-phenethyl-6-thioxanthine **106802-46-4P**, Choline, compound with 1-methyl-3-(2-methylallyl)-6-thioxanthine **878790-85-3P**, Xanthine, 1,3,8-trimethyl-6-thio-, compound with choline **878790-86-4P**, Xanthine, 1-ethyl-3-methyl-6-thio-, compound with choline **878790-87-5P**, Xanthine, 1,3-dipropyl-6-thio-, compound with choline **878794-41-3P**, Theophylline, 6-thio-, compound with choline **879632-11-8P**, Xanthine, 3-allyl-1-ethyl-6-thio-, compound with choline
RL: PREP (Preparation)
(preparation of)

RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



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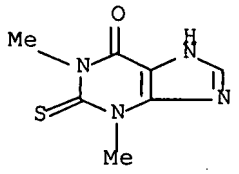

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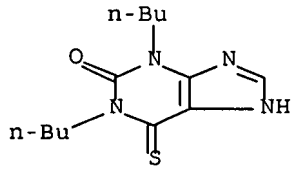

RN 42458-87-7 CAPLUS
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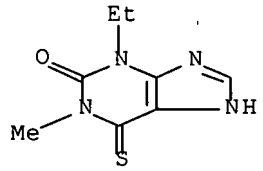

RN 42458-88-8 CAPLUS
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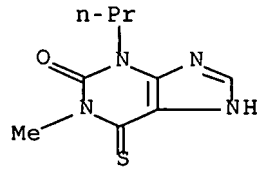

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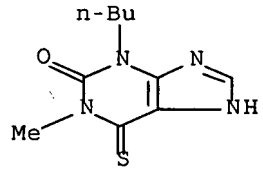

RN 42458-91-3 CAPLUS
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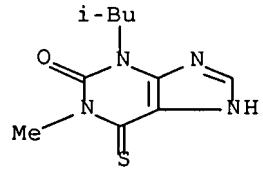

RN 42458-92-4 CAPLUS
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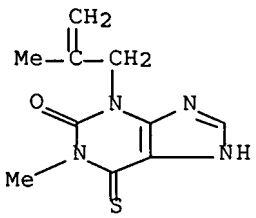

RN 42458-93-5 CAPLUS
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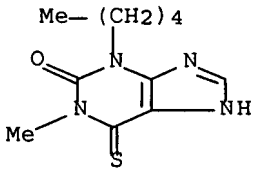

RN 42458-94-6 CAPLUS
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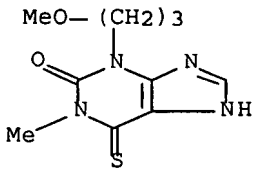

RN 42458-95-7 CAPLUS
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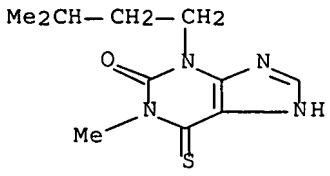

RN 42458-96-8 CAPLUS
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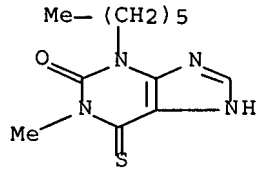

RN 42458-97-9 CAPLUS
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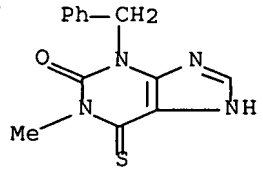

RN 42458-98-0 CAPLUS
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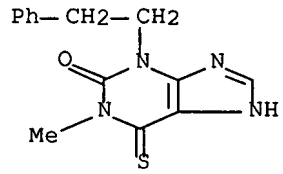

RN 42458-99-1 CAPLUS
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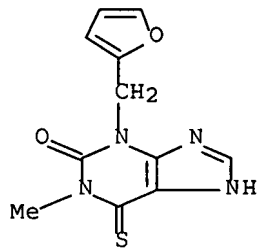

RN 42459-00-7 CAPLUS
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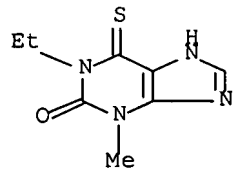

RN 42459-01-8 CAPLUS
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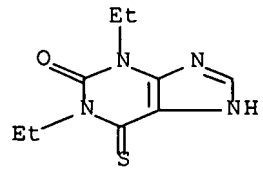

RN 42459-02-9 CAPLUS
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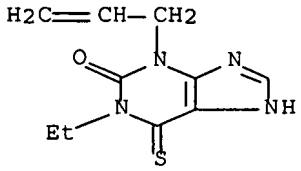

RN 42459-03-0 CAPLUS
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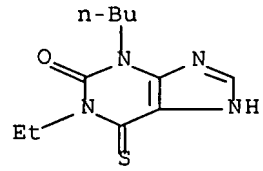

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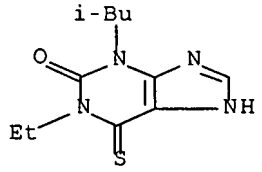

RN 42459-06-3 CAPLUS
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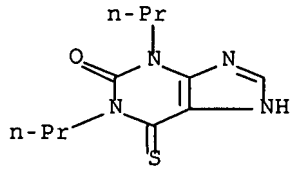
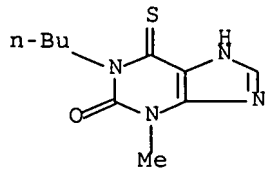
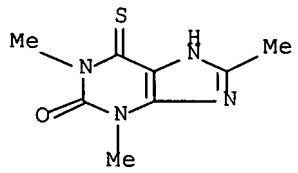


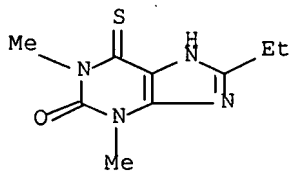
RN 42459-07-4 CAPLUS
CN 2H-Purin-2-one, 1-butyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 42459-09-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3,8-trimethyl-6-thioxo- (9CI) (CA INDEX NAME)



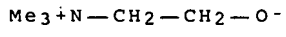
RN 42459-10-9 CAPLUS
CN 2H-Purin-2-one, 8-ethyl-1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 90230-11-8 CAPLUS
CN Choline, compd. with 6-thiotheophylline (6CI, 7CI) (CA INDEX NAME)

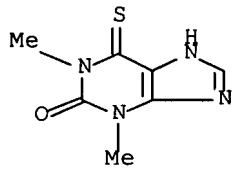
CM 1

CRN 44519-34-8
CMF C5 H13 N O

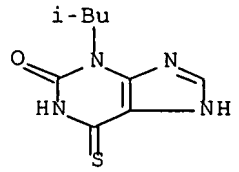


CM 2

CRN 2398-70-1
CMF C7 H8 N4 O S



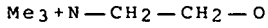
RN 93263-24-2 CAPLUS
CN Xanthine, 3-isobutyl-6-thio- (7CI) (CA INDEX NAME)



RN 96536-20-8 CAPLUS
CN Choline, compd. with 3-ethyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

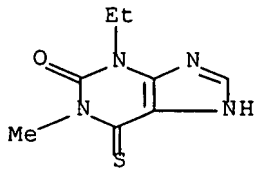
CM 1

CRN 44519-34-8
CMF C5 H13 N O



CM 2

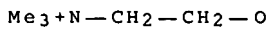
CRN 42458-87-7
CMF C8 H10 N4 O S



RN 96536-21-9 CAPLUS
CN Choline, compd. with 1,3,8-trimethyl-6-thioxanthine (7CI) (CA INDEX NAME)

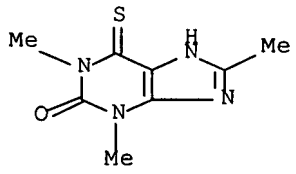
CM 1

CRN 44519-34-8
CMF C5 H13 N O



CM 2

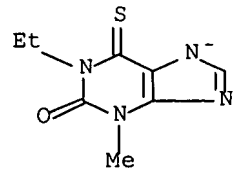
CRN 42459-09-6
CMF C8 H10 N4 O S



RN 96652-89-0 CAPLUS
CN Choline, compd. with 1-ethyl-3-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

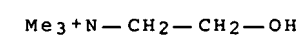
CM 1

CRN 96652-88-9
CMF C8 H9 N4 O S



CM 2

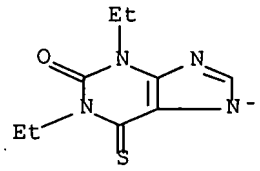
CRN 62-49-7
CMF C5 H14 N O



RN 96986-49-1 CAPLUS
CN Choline, compd. with 1,3-diethyl-6-thioxanthine (7CI) (CA INDEX NAME)

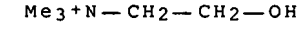
CM 1

CRN 96986-48-0
CMF C9 H11 N4 O S



CM 2

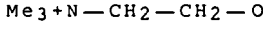
CRN 62-49-7
CMF C5 H14 N O



RN 97212-72-1 CAPLUS
CN Choline, compd. with 1-methyl-3-propyl-6-thioxanthine (7CI) (CA INDEX NAME)

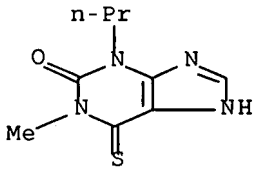
CM 1

CRN 44519-34-8
CMF C5 H13 N O



CM 2

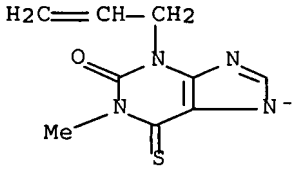
CRN 42458-88-8
CMF C9 H12 N4 O S



RN 97282-72-9 CAPLUS
CN Choline, compd. with 3-allyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

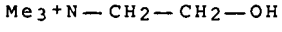
CM 1

CRN 97282-71-8
CMF C9 H9 N4 O S



CM 2

CRN 62-49-7
CMF C5 H14 N O

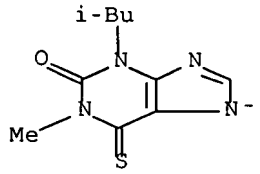


RN 97406-00-3 CAPLUS
CN Choline, compd. with 3-isobutyl-1-methyl-6-thioxanthine (6CI, 7CI) (CA INDEX NAME)

CM 1

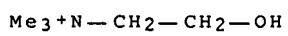
CRN 97405-99-7

CMF C10 H13 N4 O S



CM 2

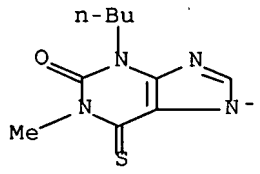
CRN 62-49-7
CMF C5 H14 N O



RN 97406-02-5 CAPLUS
CN Choline, compd. with 3-butyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

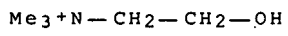
CM 1

CRN 97406-01-4
CMF C10 H13 N4 O S



CM 2

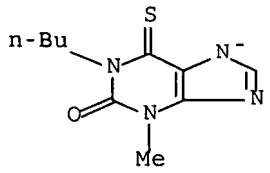
CRN 62-49-7
CMF C5 H14 N O



RN 97439-87-7 CAPLUS
CN Choline, compd. with 1-butyl-3-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

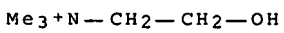
CM 1

CRN 97439-86-6
CMF C10 H13 N4 O S



CM 2

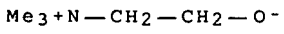
CRN 62-49-7
CMF C5 H14 N O



RN 97616-67-6 CAPLUS
CN Choline, compd. with 3-butyl-1-ethyl-6-thioxanthine (7CI) (CA INDEX NAME)

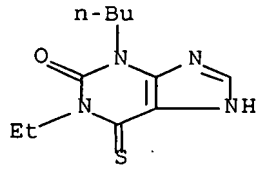
CM 1

CRN 44519-34-8
CMF C5 H13 N O



CM 2

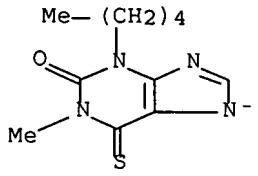
CRN 42459-03-0
CMF C11 H16 N4 O S



RN 97767-38-9 CAPLUS
CN Choline, compd. with 1-methyl-3-pentyl-6-thioxanthine (7CI) (CA INDEX NAME)

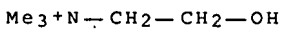
CM 1

CRN 97767-37-8
CMF C11 H15 N4 O S



CM 2

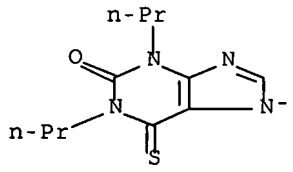
CRN 62-49-7
CMF C5 H14 N O



RN 97767-40-3 CAPLUS
CN Choline, compd. with 1,3-dipropyl-6-thioxanthine (7CI) (CA INDEX NAME)

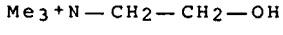
CM 1

CRN 97767-39-0
CMF C11 H15 N4 O S



CM 2

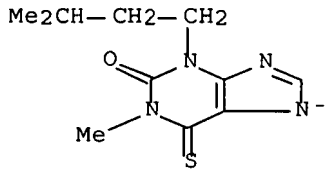
CRN 62-49-7
CMF C5 H14 N O



RN 97783-97-6 CAPLUS
CN Choline, compd. with 3-isopentyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

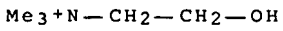
CM 1

CRN 97783-96-5
CMF C11 H15 N4 O S



CM 2

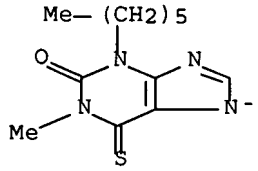
CRN 62-49-7
CMF C5 H14 N O



RN 98174-21-1 CAPLUS
CN Choline, compd. with 3-hexyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

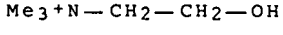
CM 1

CRN 98174-20-0
CMF C12 H17 N4 O S



CM 2

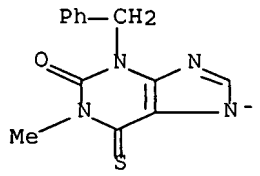
CRN 62-49-7
CMF C5 H14 N O



RN 98801-33-3 CAPLUS
CN Choline, compd. with 3-benzyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 98801-32-2
CMF C13 H11 N4 O S



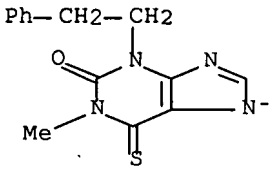
CM 2

CRN 62-49-7
CMF C5 H14 N O

RN 99688-81-0 CAPLUS
CN Choline, compd. with 1-methyl-3-phenethyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 99688-80-9
CMF C14 H13 N4 O S



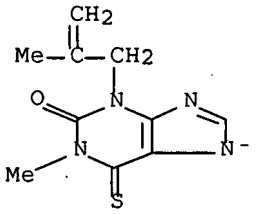
CM 2

CRN 62-49-7
CMF C5 H14 N O

RN 106802-46-4 CAPLUS
CN Choline, compd. with 1-methyl-3-(2-methylallyl)-6-thioxanthine (7CI) (CA INDEX NAME)

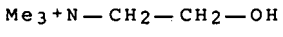
CM 1

CRN 106802-45-3
CMF C10 H11 N4 O S



CM 2

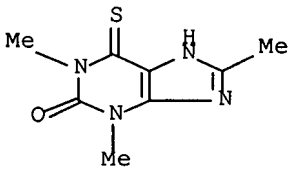
CRN 62-49-7
CMF C5 H14 N O



RN 878790-85-3 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3,8-trimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

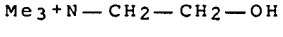
CM 1

CRN 42459-09-6
CMF C8 H10 N4 O S



CM 2

CRN 62-49-7
CMF C5 H14 N O

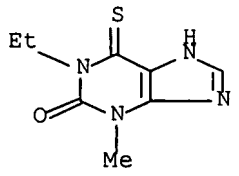


RN 878790-86-4 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1-ethyl-1,3,6,7-

tetrahydro-3-methyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

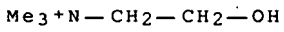
CM 1

CRN 42459-00-7
CMF C8 H10 N4 O S



CM 2

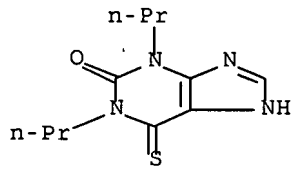
CRN 62-49-7
CMF C5 H14 N O



RN 878790-87-5 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

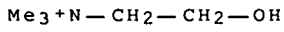
CM 1

CRN 42459-06-3
CMF C11 H16 N4 O S



CM 2

CRN 62-49-7
CMF C5 H14 N O

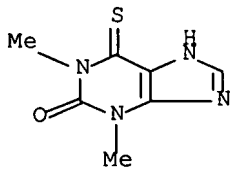


RN 878794-41-3 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

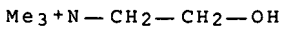
CM 1

CRN 2398-70-1
CMF C7 H8 N4 O S



CM 2

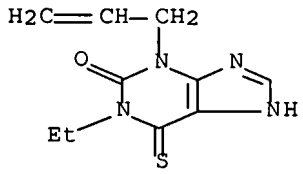
CRN 62-49-7
CMF C5 H14 N O



RN 879632-11-8 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1-ethyl-1,3,6,7-tetrahydro-3-(2-propenyl)-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

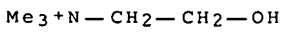
CM 1

CRN 42459-02-9
CMF C10 H12 N4 O S

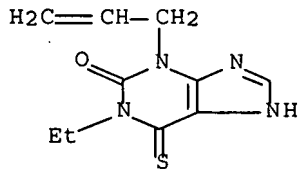


CM 2

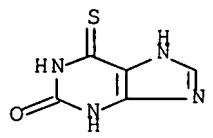
CRN 62-49-7
CMF C5 H14 N O



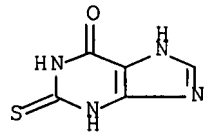
IT **42459-02-9**, Xanthine, 3-allyl-1-ethyl-6-thio-
(sodium derivative, blood-vessel and bronchial dilation by)
RN 42459-02-9 CAPLUS
CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-(2-propenyl)-6-thioxo- (9CI) (CA INDEX NAME)



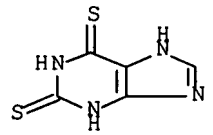
L57 ANSWER 101 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:418827 CAPLUS Full-text
DOCUMENT NUMBER: 57:18827
ORIGINAL REFERENCE NO.: 57:3862h-i,3863a
TITLE: Specific reactions of the purine-oxidizlng system of Pseudomonas aeruginosa
AUTHOR(S): Bergmann, Felix; UngarWaron, Hanna; Kwietny-Govrin, Hanna; Goldberg, Hilda; Leon, Shalom
CORPORATE SOURCE: Hebrew Univ., Jerusalem, Israel
SOURCE: Biochimica et Biophysica Acta, Specialized Section on Nucleic Acids and Related Subjects (1962), 55, 512-22
CODEN: BBASB7; ISSN: 0926-6550
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 22 Apr 2001
AB cf. CA 55, 26059g. Resting cells of -P. aeruginosa oxidized 2-aminopurine and its MeNH- and Me2N- analogs at C-8 in contrast to the action of mammalian xanthine oxidase. 6-Mercaptopurine was attacked 1st at C-2, then at C-8, and then further. This compound did not inhibit growing P. aeruginosa, but increased production of xanthine oxidase. The 3-Me derivs. of thioxanthines were oxidized at C-8, while 3methylhypoxanthine was first attacked at C-2. The resulting complex, containing 3-methylxanthine, dissociated before further oxidation to 3-methyluric acid, in contrast to xanthine. The results are discussed in reference to the mechanism of attack and the different actions of bacterial and mammalian xanthine oxidases. 21 references.
IT **2002-59-7**, Xanthine, 6-thio- **2487-40-3**, Xanthine, 2-thio- **5437-25-2**, Xanthine, dithio- **28139-02-8**, Xanthine, 3-methyl-2-thio- **33285-76-6**, Xanthine, 3-methyl-6-thio- **33285-77-7**, Xanthine, 3-methyl-2,6-dithio-
(oxidation by xanthine oxidase of Pseudomonas aeruginosa)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



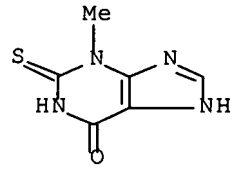
RN 2487-40-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- (9CI) (CA INDEX NAME)



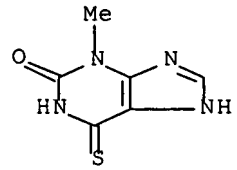
RN 5437-25-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



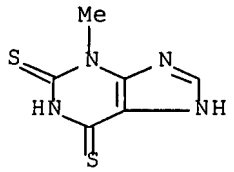
RN 28139-02-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 33285-77-7 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



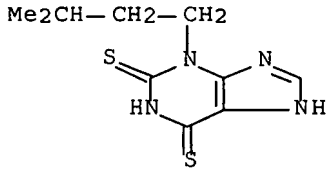
L57 ANSWER 102 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:410979 CAPLUS Full-text
DOCUMENT NUMBER: 57:10979
ORIGINAL REFERENCE NO.: 57:2268g-i,2269a-i,2270a-c
TITLE: Alkaloids of Tylophora crebriflora-structure and synthesis of tylocrebrine, a new phenanthroindolizidine alkaloid
AUTHOR(S): Gellert, E.; Govindachari, T. R.; Lakshmikantham, M. V.; Ragade, I. S.; Rudzats, R.; Viswanathan, N.
CORPORATE SOURCE: Univ. N. S. W., Sydney
SOURCE: Journal of the Chemical Society (1962) 1008-14
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB Milled T. crebrifiora (21 lb.) extracted with hot MeOH, the extract concentrated to small volume (4 1.), diluted with 2 1. H2O, concd, to 800 ml. in a climbing film evaporator, and the mixture filtered while warm gave a solid (I) and a filtrate (II). II acidified with dilute AcOH, extracted exhaustively with CCl4, the combined CCl4 solns, extracted with 2N HCl, the extract combined with the previous acidic phase, and filtered gave a filtrate (III), which gave a strong Mayer test and showed 2 fluorescent spots when chromatographed on paper in BuOH-AcOH (Rf 0.2 and 0.5). I in warm 2N AcOH diluted with hot H2O, cooled, filtered, the filtrate extracted with CCl4, combined with III, made basic with concd, aqueous, the precipitate (45 g.) repeatedly precipitated from hot aqueous AcOH with concd, aqueous NH3, extracted (Soxhlet) with MeOH, and the product crystd, from MeOH gave crude alkaloid mixture (IV). Crude IV (in 2 g. batches) subjected to partition chromatography in 15:85 PrOH-2N-AcOH on a cellulose column (partial separation into fractions with Rf 0.2 and 0.5), the fractions from several such chromatograms combined (intermediate fractions were rechromatographed), the 1st fraction evaporated in vacuo, the residue dissolved in warm dilute AcOH, made alkaline with concd, aqueous NH3 and the crude alkaloid [Rf 0.5 (in 3:97 AcOH-BuOH saturated with H2O) (solvent A)] crystallized 3 times from MeOH gave tylocrebrine (V), m. 218-20° (decomposition), λ 263, 342, and 360 mμ (ε 4.81, 3.25, and 3.09), [α]24D -45 ± 2° (c 0.74, CHCl3), pKa 6.7 (in 50% aqueous EtOH) [HI salt m. 214-17° (decomposition) (aqueous MeOH); perchlorate m. 262-4° (decomposition); picrate m. 134-6° (Me2CO containing a little MeOH)]. The crude alkaloid [Rf 0.2 (solvent A)] from the 2nd fraction recrystd. 3 times from CHCl3-MeOH gave tylophorine (isomeric with V), m. 282-4° (decomposition), λ 257, 290, 340, 355 mμ (ε 4.82, 4.51, 3.43, 2.96). V refluxed on a H2O bath with excess MeI in MeOH until dissolved, then refluxed 30 min. more, concentrated, and cooled gave optically active V.MeI, m. 255-8° (decomposition) (MeOH), [α]21D -30 ± 2° (c 0.30, MeOH). Optically active V.MeI refluxed 30 min. in 20% aqueous NaOH gave (±)-V.MeI, m. 264-6° (decomposition) (MeOH), [α]21D 0° (c 0.10, MeOH). V.MeI (1.4 g.) refluxed with AgCl in aqueous MeOH, the resulting V.MeCl shaken with Ag2O in H2O, the solution of V.MeOH evaporated to dryness, the residue heated 3 min. at

240°/0.2 mm., and the product chromatographed in C6H6 on basic Al2O3 gave 400 mg. VI, m. 144.5-5.0° (C6H6-petr. ether, then petr. ether). V.MeI (100 mg.) converted directly into V.MeOH (with Ag2O in 10 ml. H2O; 5 hr.), the mixture filtered, the filtrate evaporated in vacuo at 50° the residue heated 30 min. at 100°/0.05 mm., the product repeatedly extracted with hot C6H6, and chromatographed in C6H6 on Al2O3 gave 10 mg. VI, m. 144.5-5.0°. VI (50 mg.) in 3 ml. AcOH heated 5 min. at 125° with excess HIO4 gave no CH2O (no precipitate with dimedon). Et 3,4,6,7-tetramethoxyphenanthrene-9-carboxylate (3 g.) in 25 ml. dry tetrahydrofuran added to 1.5 g. LiAlH4 in 15 ml. tetrahydrofuran with stirring, stirred 4 hrs., treated with Et2O and H2O, the organic layer decanted, and evaporated gave 2.2 g. 9 - hydroxymethyl - 3,4,6,7 - tetramethoxyphenanthrene (VII), m. 164-5° (C6H6). VII (5 g.), 4 ml. SOCl2, and 0.5 ml. pyrldine in 120 ml. CHCl3 heated 15 min. at 40-60°, cooled, poured into H2O, extracted with CHCl3, the extract dried, concentrated to small volume, and diluted with petr. ether gave 4.2 g. 9-chloromethyl-3,4,6,7-tetramethoxyphenanthrene (VIII), m. 148° (decomposition) (C6H6-petr. ether). VIII (4 g.) in 40 ml. dry tetrahydrofuran added dropwise with stirring to pyrrylmagnesium bromide (from 1.8 g. Mg, 5.8 ml. EtBr, and 5.26 ml. freshly distilled pyrrole) in Et2O cooled in ice under N, stirred 3 hrs. during which the mixture was allowed to reach room temperature, diluted with Et2O, decomposed with saturated aqueous NH4Cl, the organic layer separated, washed with H2O, dried, evaporated, and the residue chromatographed in CHCl3 on Al2O3 gave 2 g. 2-(3,4,6,7-tetramethoxy-9- phenanthrylmethyl)pyrrole (IX), m. 155-6° (C6H6-petr. ether). IX (0.4 g.) in 30 ml. AcOH containing 0.25 g. PtO2 hydrogenated 8 hrs. at room temperature at 60 lb./sq, in., filtered, the filtrate evaporated in vacuo, the residue extracted repeatedly with hot dilute HCl, the combined exts. basified with aqueous NH3, and the product isolated with CHCl3 gave 0.25 g. corresponding pyrrolidine (X), oil; picrate m. 247-9° (AcOH). X (0.5 g.) and 3 ml. 98% HCO2H heated 1.5 hrs. at 180°, cooled, dissolved in CHCl3, the solution washed, dried, evaporated, the residual N-formyl derivative refluxed 1.5 hrs. with 4 ml. POCl3 and 15 ml. PhMe, the solution mixture cooled, diluted with petr. ether, the resulting quaternary chloride dried in vacuo, reduced with 0.8 g. NaBH4 in 30 ml. MeOH, the solution evaporated in vacuo, the residue taken up in CHCl3, the solution washed with H2O, dried, evaporated, and the residue chromatographed in CHCl3 on Al2O3 gave 0.2 g. (±)-V, m. 219-21° (CHCl3-MeOH). (±)-V (200 mg.) in 10 ml. CHCl3 refluxed 3 hrs. on a H2O bath with 2 ml. MeI and kept overnight at 30°, the solution evaporated, the resulting (±)-V.MeI shaken 5 hrs. with Ag2O (from 1 g. AgNO3) and 10 ml. H2O, and the (±)-V.MeOH subjected to Hofmann degradation as above gave 40 mg. VI, m. 144.5-5.0° (C6H6-petr. ether). 2-Amino-α-(3,4- dimethoxyphenyl)-4,5-dimethoxycinnamic acid (G. et al., loc. cit.) diazotized in Me2CO with BuONO and subjected to Pschorr ring closure gave 2,3,5,6-tetramethoxyphenanthrene-9-carboxylic acid (XI). XI (5 g.) refluxed 4 hrs. with 4 ml. concentrated H2SO4 in 150 ml. MeOH gave 4.2 g. Me ester of XI, m. 150° (EtOH). XI was converted successively as above into 9-hydroxymethyl-2,3,5,6-tetramethoxyphenanthrene, m. 133° (C6H6); 9 - chloromethyl - 2,3,5,6 - tetramethoxyphenanthrene, m. 163-4° (C6H6-petr. ether); 2-(2,3,5,6-tetramethoxy-9- phenanthrylmethyl)pyrrolidine [picrate m. 218° (decomposition) (AcOH-EtOH)]; and finally 9,11,12,13,13a, 14-hexahydro3,4,6,7- tetramethoxydibenzo [f,h] pyrrolo [1,2-b] isoquinoline (XII), m. 219° (CHCl-MeOH). XII (200 mg.) converted to the methiodide and the product subjected to the Hofmann degradation as above gave 30 mg. XIII, m. 137-8° (C6H6-petr. ether). The structure of V is shown.

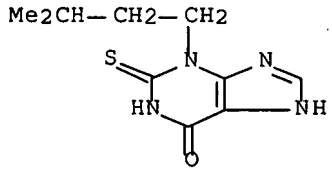
IT **32051-91-5P**, Xanthine, 3-isopentyl-2,6-dithio- **94689-49-3P**
, Xanthine, 3-isopentyl-2-thio-
RL: PREP (Preparation)
(preparation of)

RN 32051-91-5 CAPLUS

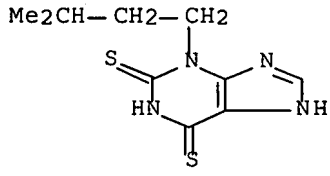
CN Xanthine, 3-isopentyl-2,6-dithio- (7CI, 8CI) (CA INDEX NAME)



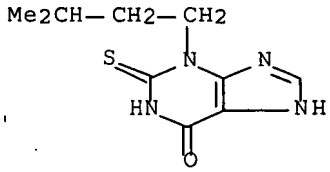
RN 94689-49-3 CAPLUS
CN Xanthine, 3-isopentyl-2-thio- (7CI) (CA INDEX NAME)



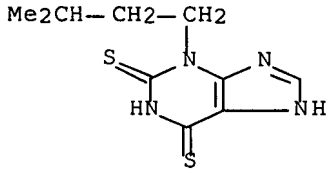
L57 ANSWER 103 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:410978 CAPLUS Full-text
DOCUMENT NUMBER: 57:10978
ORIGINAL REFERENCE NO.: 57:2268g
TITLE: Synthesis of Dihydrotriacanthine
AUTHOR(S): Leonard, Nelson J.; Laursen, Richard A.
CORPORATE SOURCE: Univ. of Illinois, Urbana
SOURCE: Journal of Organic Chemistry (1962), 27, 1778-80
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB 3-Isopentyladenine was synthesized and shown to be identical with dihydrotriacan thine.
IT **32051-91-5P**, Xanthine, 3-isopentyl-2,6-dithio- **94689-49-3P**, Xanthine, 3-isopentyl-2-thio-
RL: PREP (Preparation)
(preparation of)
RN 32051-91-5 CAPLUS
CN Xanthine, 3-isopentyl-2,6-dithio- (7CI, 8CI) (CA INDEX NAME)



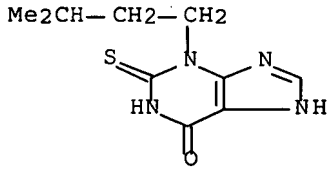
RN 94689-49-3 CAPLUS
CN Xanthine, 3-isopentyl-2-thio- (7CI) (CA INDEX NAME)



L57 ANSWER 104 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:410977 CAPLUS Full-text
DOCUMENT NUMBER: 57:10977
ORIGINAL REFERENCE NO.: 57:2267f-i,2268f-g
TITLE: Synthesis of calycotomine and its analogs
AUTHOR(S): Chatterjee, A.; Chaudhury, N. Aditya
CORPORATE SOURCE: Univ. Coll. Sci., Calcutta
SOURCE: Journal of Organic Chemistry (1962), 27, 309-10
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB cf. CA 54, 22693g. Liquid NH3 (300 ml.) containing 8.73 g. Na treated with a thin stream of 22.0 g. 3,4-(MeO)2C6H3CH2CH2NH2 and the mixture kept 6 hrs. with rise of temperature to 30° decompd, by cautious addition of ice and washed twice with 50 ml. Et2O, the aqueous phase aerated and the NH3-free solo. acidified with AcOH with cooling, washed with Et2O and made alkaline with NaHCO3, extracted 3 times with 100 ml. BuOH and the dried extract (150 ml.) treated with HCl in Et2O yielded 18.0 g. 3,4-HO(MeO)C6H3CH2CH2NH2.HCl (I), m. 203-4° (absolute alc.Et2O). I (0.9 g.) and 0.4 g. HOCH2CHO in 10 ml. H2O adjusted to pH 4.,5-5.0 and kept 3 days at 30° basified with Na2CO3 and extracted with CHCI3 gave 0.6 g. 6-demethylcalycotomine (II, R1 = OH, R2 = OMe) (III), m. 198-200° (decomposition). III (0.6 g.) in 50 ml. dry Et2O added slowly to CH2N2 [from Me(NO)NCONH2] and kept 16 hrs. at 28-6° before evapn, in vacuo, the residue (0.5 g.) taken up in 20 ml. 4N HCl and washed 3 times with 25 ml. Et2O, the acidic aqueous solution basified with 45 ml. 10% aqueous NaOH and extracted 3 times with 50 ml. CHCl3 yielded 45-50% dl-calycotomine (II, R1 = R2 - OMe), m. 134° (1:1 EtOAc-petr. ether), λ 240, 290 mμ (log ε 3.48, 3.66, alc.); HCl salt m. 195-6° (absolute alc.-Et2O). Concentrated HCl (8 ml.) heated 8 hrs. with 5.0 g. 3,4-(MeO)2C6H3CH2CH2NH2 at 160-70° in a sealed tube and the product cooled in an ice bath yielded 4.0 g. 3,4-(HO)2C6H3CH2NH2HCl (IV), m. 241° (Me2CO). IV (1.0 g.) and 0.6 g. HOCH2CHO in 10 ml. H2O adjusted to pH 3-4 and kept 3 days at 25-6°, concd, in vacuo and the cryst, product recrystd, from 1: 1 alc.-Me2CO gave 0.85 g. 6,7-demethylcalycotomine (II, R1 = R2 = OH), m. 208-9° (decomposition), λ 288 mμ (log ε 3.57). Condensation of 0.08 g. with 0.15 g. 3,4-(HO)2C6H3CH2CH(NH2)CO2H.HCl in 5 ml. H2O at pH 4-5 gave 0.1 g. 3-carboxy-6,7-demethylealycotomine, m. 281-2° (decomposition), λ 280 mμ (log ε 3.54).
IT **32051-91-5P**, Xanthine, 3-isopentyl-2,6-dithio- **94689-49-3P**, Xanthine, 3-isopentyl-2-thio-
RL: PREP (Preparation)
(preparation of)
RN 32051-91-5 CAPLUS
CN Xanthine, 3-isopentyl-2,6-dithio- (7CI, 8CI) (CA INDEX NAME)



RN 94689-49-3 CAPLUS
CN Xanthine, 3-isopentyl-2-thio- (7CI) (CA INDEX NAME)

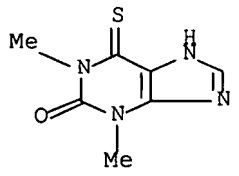


L57 ANSWER 105 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:66964 CAPLUS
DOCUMENT NUMBER: 56:66964
ORIGINAL REFERENCE NO.: 56:12912a-c
TITLE: N-Alkyl thiopurines
PATENT ASSIGNEE(S): Wellcome Foundation Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

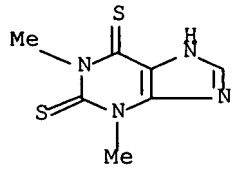
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 887409		19620117	GB 1958-17890	19580604 <--
PRIORITY APPLN. INFO.:			US	19570606 <--

ED Entered STN: 22 Apr 2001
AB The title compds., which increase the flow of blood in coronary vessels, were prepared by treating an N-alkoxypurine with P2S5 at 115-200° in an inert solvent. Thus, 4.3 g. 3-methylhypoxanthine, 12 g. P2O5, and 100 ml. pyridine was refluxed 2.5 hrs., the pyridine removed under reduced pressure, and the residue heated with 200 ml. water 20 min. to give 3-methyl-6-thiohypoxanthine (3.25 g. crude), m. 322-3° (H2O), λ242, 335 mμ (pH 1) and 242, 333 mμ (pH 11). Theophylline (I) (10 g.), 50 g. P2S5, and 150 ml. tetrahydronaphthalene heated 5 hrs. at 190° gave 1,3-dimethyl-2,6-dithioxanthine (5.2 g.), m. 252-4° (95% alc.), λ 252, 297, 345 mμ (pH 1) and 265, 295, 345 mμ (pH 11). I (5 g.) and 15 g. P2S5 refluxed 2 hrs. in 150 ml. pyridine gave 1,3-dimethyl-6-thioxanthine, m. 315-17° (95% alc.), λ 270, 342 mμ (pH 1) and 260, 340 mμ (pH 11). Similarly prepared were 3-methyl-6-thioxanthine, m. 320°, λ 345 mμ (pH 1) and 337 mμ (pH 11), and 3-methyl-2,6-dithioxanthine, m. 340°, λ 254, 298, 352 mμ (pH 1) and 257, 302,342 mμ (pH 11).
IT **2398-70-1P**, Theophylline, 6-thio- **6501-94-6P**, Theophylline, dithio- **33285-76-6P**, Xanthine, 3-methyl-6-thio- **33285-77-7P**, Xanthine, 3-methyl-2,6-dithio-
RL: PREP (Preparation)
(preparation of)

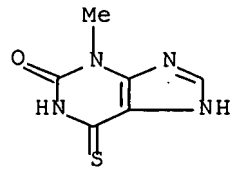
RN 2398-70-1 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo- (9CI) (CA INDEX NAME)



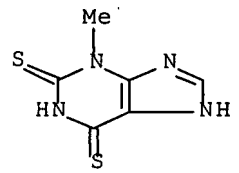
RN 6501-94-6 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)



RN 33285-77-7 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L57 ANSWER 106 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:41798 CAPLUS Full-text
DOCUMENT NUMBER: 56:41798

ORIGINAL REFERENCE NO.: 56:7935c-f
TITLE: Structure-activity relations in a series of 6-thioxanthines with bronchodilator and coronary dilator properties
AUTHOR(S): Armitage, A. K.; Boswood, Janet; Large, B. J.
SOURCE: British Journal of Pharmacology and Chemotherapy (1961), 17, 196-207
CODEN: BJPCAL; ISSN: 0366-0826
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB The bronchodilator, coronary dilator, central stimulant, and diuretic activities of forty-seven 1,3-and 3,7-disubstituted and 1,3,7-trisubstituted 6-thioxanthines are reported. Bronchodilator activity was determined on the isolated guinea pig tracheal ring prepns. and coronary dilator activity on the dog heart-lung prepns. Diuretic activity was determined using conscious rats, and stimulant activity using mice. The in vivo bronchodilatory activity was determined by the protection afforded to guinea pigs against bronchoconstrictor aerosol. While choline 6-thiotheophyllinate is twice as active as choline theophyllinate as a broncho- and coronary dilator, several higher members of the theophylline series are more active than the 6-thio analogs. The 6-thiotheophylline is more active than the 6-thiotheobromine and 6-thiocaffeine. The 1,3-disubstituted compds. were more active as broncho- and coronary dilators than the 3,7-substituted compds. Maximum bronchodilator activity was achieved with relatively large alkyl groups in the 1 and 3 positions, and the 3-isobutyl derivative of 1-methyl-6-thiotheophylline was most active. Large groups in the 1-position may reduce oral absorption. Compds. with unsatd. or substituted alkyl groups in the 3-position are less bronchoactive than compds. containing the corresponding saturated or unsubstituted groups. A 1-methyl group may be essential for coronary dilator activity. All the compds. tested had low diuretic activity. 6-Thiocaffeines, in contrast to caffeine, show no stimulant properties.
IT **90230-11-8**, Choline, compound with 6-thiotheophylline
96536-20-8, Choline, compound with 3-ethyl-1-methyl-6-thioxanthine
96536-21-9, Choline, compound with 1,3,8-trimethyl-6-thioxanthine
96652-89-0, Choline, compound with 1-ethyl-3-methyl-6-thioxanthine
96986-49-1, Choline, compound with 1,3-diethyl-6-thioxanthine
97212-71-0, Choline, compound with 8-ethyl-6-thiotheophylline
97212-72-1, Choline, compound with 1-methyl-3-propyl-6-thioxanthine
97282-72-9, Choline, compound with 3-allyl-1-methyl-6-thioxanthine
97406-00-3, Choline, compound with 3-isobutyl-1-methyl-6-thioxanthine **97406-02-5**, Choline, compound with 3-butyl-1-methyl-6-thioxanthine **97439-87-7**, Choline, compound with 1-butyl-3-methyl-6-thioxanthine **97616-67-6**, Choline, compound with 3-butyl-1-ethyl-6-thioxanthine **97767-38-9**, Choline, compound with 1-methyl-3-pentyl-6-thioxanthine **97767-40-3**, Choline, compound with 1,3-dipropyl-6-thioxanthine **97783-97-6**, Choline, compound with 3-isopentyl-1-methyl-6-thioxanthine **98174-21-1**, Choline, compound with 3-hexyl-1-methyl-6-thioxanthine **98801-33-3**, Choline, compound with 3-benzyl-1-methyl-6-thioxanthine **99688-81-0**, Choline, compound with 1-methyl-3-phenethyl-6-thioxanthine **106802-46-4**, Choline, compound with 1-methyl-3-(2-methylallyl)-6-thioxanthine
(blood vessel and bronchial dilation by)
RN 90230-11-8 CAPLUS
CN Choline, compd. with 6-thiotheophylline (6CI, 7CI) (CA INDEX NAME)

CM 1

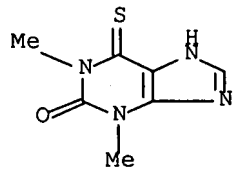
CRN 44519-34-8

CMF C5 H13 N O

$Me_3{}^+N—CH_2—CH_2—O^-$

CM 2

CRN 2398-70-1
CMF C7 H8 N4 O S



RN 96536-20-8 CAPLUS
CN Choline, compd. with 3-ethyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

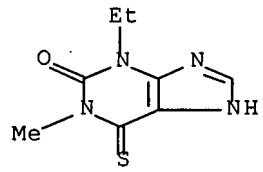
CM 1

CRN 44519-34-8
CMF C5 H13 N O

$Me_3{}^+N—CH_2—CH_2—O^-$

CM 2

CRN 42458-87-7
CMF C8 H10 N4 O S

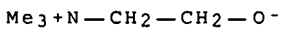


RN 96536-21-9 CAPLUS
CN Choline, compd. with 1,3,8-trimethyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

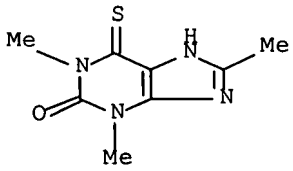
CRN 44519-34-8

CMF C5 H13 N O



CM 2

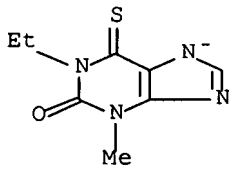
CRN 42459-09-6
CMF C8 H10 N4 O S



RN 96652-89-0 CAPLUS
CN Choline, compd. with 1-ethyl-3-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

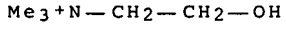
CM 1

CRN 96652-88-9
CMF C8 H9 N4 O S



CM 2

CRN 62-49-7
CMF C5 H14 N O

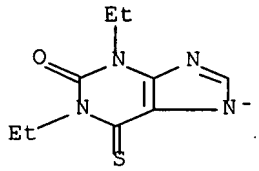


RN 96986-49-1 CAPLUS
CN Choline, compd. with 1,3-diethyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

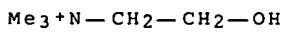
CRN 96986-48-0

CMF C9 H11 N4 O S



CM 2

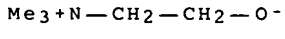
CRN 62-49-7
CMF C5 H14 N O



RN 97212-71-0 CAPLUS
CN Choline, compd. with 8-ethyl-6-thiotheophylline (7CI) (CA INDEX NAME)

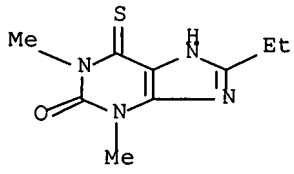
CM 1

CRN 44519-34-8
CMF C5 H13 N O



CM 2

CRN 42459-10-9
CMF C9 H12 N4 O S

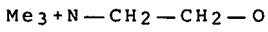


RN 97212-72-1 CAPLUS
CN Choline, compd. with 1-methyl-3-propyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

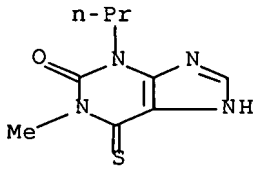
CRN 44519-34-8

CMF C5 H13 N O



CM 2

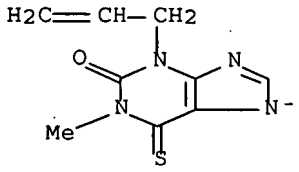
CRN 42458-88-8
CMF C9 H12 N4 O S



RN 97282-72-9 CAPLUS
CN Choline, compd. with 3-allyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

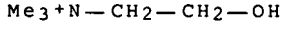
CM 1

CRN 97282-71-8
CMF C9 H9 N4 O S



CM 2

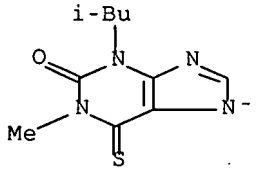
CRN 62-49-7
CMF C5 H14 N O



RN 97406-00-3 CAPLUS
CN Choline, compd. with 3-isobutyl-1-methyl-6-thioxanthine (6CI, 7CI) (CA INDEX NAME)

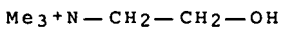
CM 1

CRN 97405-99-7
CMF C10 H13 N4 O S



CM 2

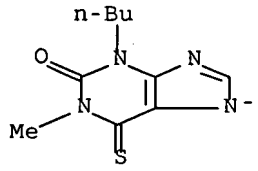
CRN 62-49-7
CMF C5 H14 N O



RN 97406-02-5 CAPLUS
CN Choline, compd. with 3-butyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

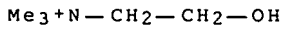
CM 1

CRN 97406-01-4
CMF C10 H13 N4 O S



CM 2

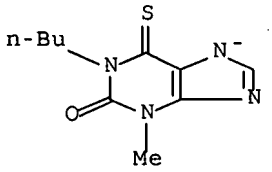
CRN 62-49-7
CMF C5 H14 N O



RN 97439-87-7 CAPLUS
CN Choline, compd. with 1-butyl-3-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

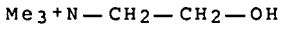
CM 1

CRN 97439-86-6
CMF C10 H13 N4 O S



CM 2

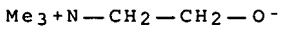
CRN 62-49-7
CMF C5 H14 N O



RN 97616-67-6 CAPLUS
CN Choline, compd. with 3-butyl-1-ethyl-6-thioxanthine (7CI) (CA INDEX NAME)

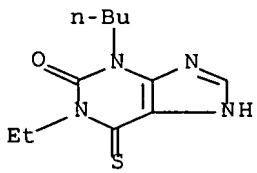
CM 1

CRN 44519-34-8
CMF C5 H13 N O



CM 2

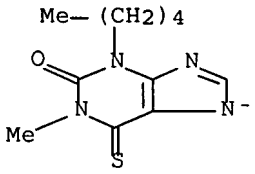
CRN 42459-03-0
CMF C11 H16 N4 O S



RN 97767-38-9 CAPLUS
CN Choline, compd. with 1-methyl-3-pentyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 97767-37-8
CMF C11 H15 N4 O S



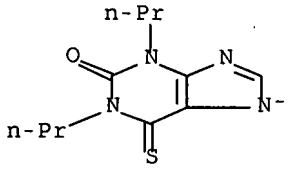
CM 2

CRN 62-49-7
CMF C5 H14 N O

RN 97767-40-3 CAPLUS
CN Choline, compd. with 1,3-dipropyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 97767-39-0
CMF C11 H15 N4 O S



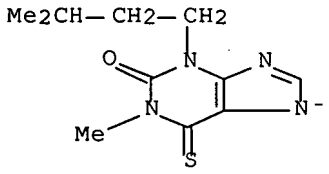
CM 2

CRN 62-49-7
CMF C5 H14 N O

RN 97783-97-6 CAPLUS
CN Choline, compd. with 3-isopentyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

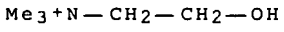
CM 1

CRN 97783-96-5
CMF C11 H15 N4 O S



CM 2

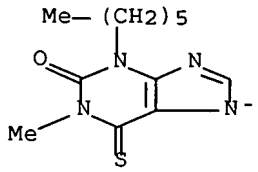
CRN 62-49-7
CMF C5 H14 N O



RN 98174-21-1 CAPLUS
CN Choline, compd. with 3-hexyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

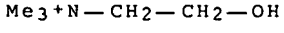
CM 1

CRN 98174-20-0
CMF C12 H17 N4 O S



CM 2

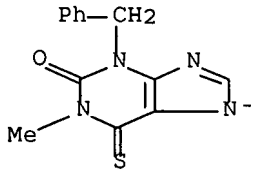
CRN 62-49-7
CMF C5 H14 N O



RN 98801-33-3 CAPLUS
CN Choline, compd. with 3-benzyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

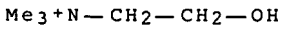
CM 1

CRN 98801-32-2
CMF C13 H11 N4 O S



CM 2

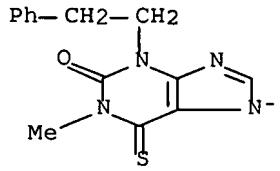
CRN 62-49-7
CMF C5 H14 N O



RN 99688-81-0 CAPLUS
CN Choline, compd. with 1-methyl-3-phenethyl-6-thioxanthine (7CI) (CA INDEX NAME)

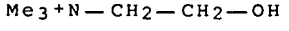
CM 1

CRN 99688-80-9
CMF C14 H13 N4 O S



CM 2

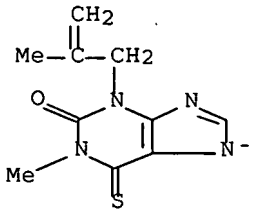
CRN 62-49-7
CMF C5 H14 N O



RN 106802-46-4 CAPLUS
CN Choline, compd. with 1-methyl-3-(2-methylallyl)-6-thioxanthine (7CI) (CA INDEX NAME)

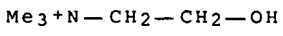
CM 1

CRN 106802-45-3
CMF C10 H11 N4 O S



CM 2

CRN 62-49-7
CMF C5 H14 N O



IT **96536-20-8**, Xanthine, 3-ethyl-1-methyl-6-thio-, compound with choline **96986-49-1**, Xanthine, 1,3-diethyl-6-thio-, compound with choline **97212-72-1**, Xanthine, 1-methyl-3-propyl-6-thio-, compound with choline **97406-02-5**, Xanthine, 3-butyl-1-methyl-6-thio-, compound with choline **97439-87-7**, Xanthine, 1-butyl-3-methyl-6-thio-, compound with choline **97616-67-6**, Xanthine, 3-butyl-1-ethyl-6-thio-, compound with choline **97767-38-9**, Xanthine, 1-methyl-3-pentyl-6-thio-, compound with choline **97783-97-6**, Xanthine, 3-isopentyl-1-methyl-6-thio-, compound with choline **98174-21-1**, Xanthine, 3-hexyl-1-methyl-6-thio-, compound with choline **98801-33-3**, Xanthine, 3-benzyl-1-methyl-6-thio-, compound with choline **99688-81-0**, Xanthine, 1-methyl-3-phenethyl-6-thio-, compound with choline **106802-46-4**, Xanthine, 1-methyl-3-(2-methylallyl)-6-thio-, compound with choline **856653-25-3**, Theophylline, 8-ethyl-6-thio-, compound with choline **878790-85-3**, Xanthine, 1,3,8-trimethyl-6-thio-, compound with choline **878790-86-4**, Xanthine, 1-ethyl-3-methyl-6-thio-, compound with choline **878790-87-5**, Xanthine, 1,3-dipropyl-6-thio-, compound with choline **878794-41-3**, Theophylline, 6-thio-, compound with choline **879632-11-8**, Xanthine, 3-allyl-1-ethyl-6-thio-, compound with choline
(blood-vessel and bronchial dilation by)

RN 96536-20-8 CAPLUS
CN Choline, compd. with 3-ethyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

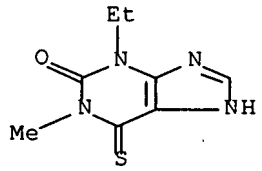
CM 1

CRN 44519-34-8
CMF C5 H13 N O

$Me_3{}^+N—CH_2—CH_2—O^-$

CM 2

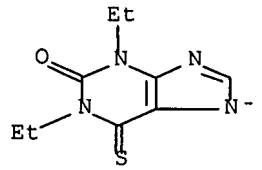
CRN 42458-87-7
CMF C8 H10 N4 O S



RN 96986-49-1 CAPLUS
CN Choline, compd. with 1,3-diethyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 96986-48-0
CMF C9 H11 N4 O S



CM 2

CRN 62-49-7
CMF C5 H14 N O

$Me_3{}^+N—CH_2—CH_2—OH$

RN 97212-72-1 CAPLUS
CN Choline, compd. with 1-methyl-3-propyl-6-thioxanthine (7CI) (CA INDEX NAME)

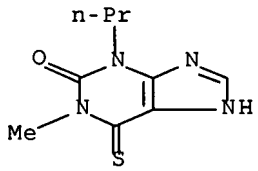
CM 1

CRN 44519-34-8
CMF C5 H13 N O

$Me_3{}^+N—CH_2—CH_2—O^-$

CM 2

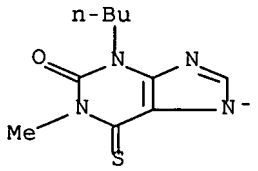
CRN 42458-88-8
CMF C9 H12 N4 O S



RN 97406-02-5 CAPLUS
CN Choline, compd. with 3-butyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

CRN 97406-01-4
CMF C10 H13 N4 O S



CM 2

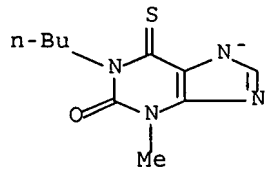
CRN 62-49-7
CMF C5 H14 N O

$Me_3{}^+N—CH_2—CH_2—OH$

RN 97439-87-7 CAPLUS
CN Choline, compd. with 1-butyl-3-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

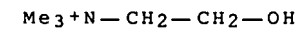
CM 1

CRN 97439-86-6
CMF C10 H13 N4 O S



CM 2

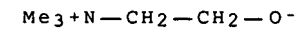
CRN 62-49-7
CMF C5 H14 N O



RN 97616-67-6 CAPLUS
CN Choline, compd. with 3-butyl-1-ethyl-6-thioxanthine (7CI) (CA INDEX NAME)

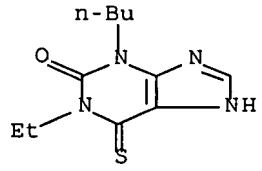
CM 1

CRN 44519-34-8
CMF C5 H13 N O



CM 2

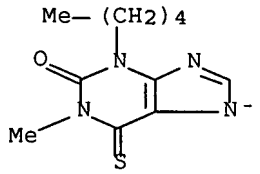
CRN 42459-03-0
CMF C11 H16 N4 O S



RN 97767-38-9 CAPLUS
CN Choline, compd. with 1-methyl-3-pentyl-6-thioxanthine (7CI) (CA INDEX NAME)

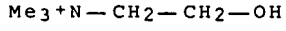
CM 1

CRN 97767-37-8
CMF C11 H15 N4 O S



CM 2

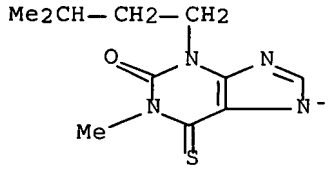
CRN 62-49-7
CMF C5 H14 N O



RN 97783-97-6 CAPLUS
CN Choline, compd. with 3-isopentyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

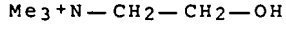
CM 1

CRN 97783-96-5
CMF C11 H15 N4 O S



CM 2

CRN 62-49-7
CMF C5 H14 N O

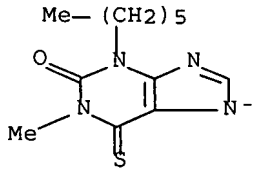


RN 98174-21-1 CAPLUS
CN Choline, compd. with 3-hexyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

CM 1

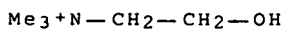
CRN 98174-20-0

CMF C12 H17 N4 O S



CM 2

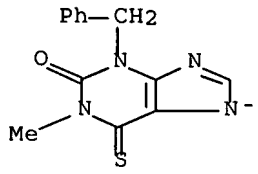
CRN 62-49-7
CMF C5 H14 N O



RN 98801-33-3 CAPLUS
CN Choline, compd. with 3-benzyl-1-methyl-6-thioxanthine (7CI) (CA INDEX NAME)

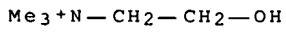
CM 1

CRN 98801-32-2
CMF C13 H11 N4 O S



CM 2

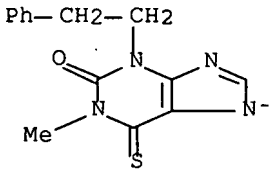
CRN 62-49-7
CMF C5 H14 N O



RN 99688-81-0 CAPLUS
CN Choline, compd. with 1-methyl-3-phenethyl-6-thioxanthine (7CI) (CA INDEX NAME)

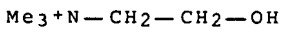
CM 1

CRN 99688-80-9
CMF C14 H13 N4 O S



CM 2

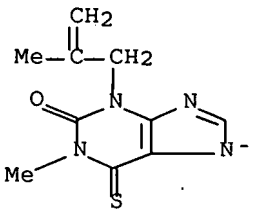
CRN 62-49-7
CMF C5 H14 N O



RN 106802-46-4 CAPLUS
CN Choline, compd. with 1-methyl-3-(2-methylallyl)-6-thioxanthine (7CI) (CA INDEX NAME)

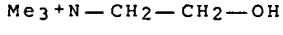
CM 1

CRN 106802-45-3
CMF C10 H11 N4 O S



CM 2

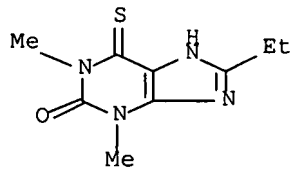
CRN 62-49-7
CMF C5 H14 N O



RN 856653-25-3 CAPLUS
CN Theophylline, 8-ethyl-6-thio-, compd. with choline (7CI) (CA INDEX NAME)

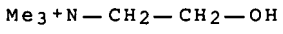
CM 1

CRN 42459-10-9
CMF C9 H12 N4 O S



CM 2

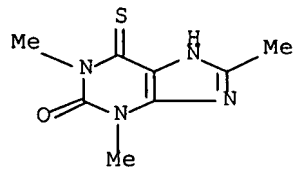
CRN 62-49-7
CMF C5 H14 N O



RN 878790-85-3 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3,8-trimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

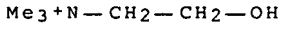
CM 1

CRN 42459-09-6
CMF C8 H10 N4 O S



CM 2

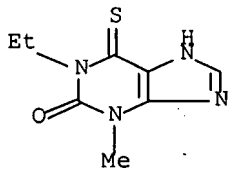
CRN 62-49-7
CMF C5 H14 N O



RN 878790-86-4 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1-ethyl-1,3,6,7-tetrahydro-3-methyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

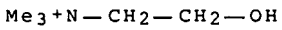
CM 1

CRN 42459-00-7
CMF C8 H10 N4 O S



CM 2

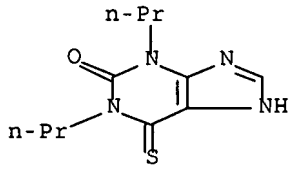
CRN 62-49-7
CMF C5 H14 N O



RN 878790-87-5 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3-dipropyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

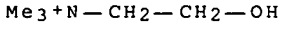
CM 1

CRN 42459-06-3
CMF C11 H16 N4 O S



CM 2

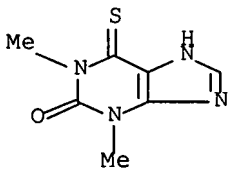
CRN 62-49-7
CMF C5 H14 N O



RN 878794-41-3 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

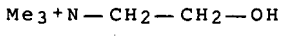
CM 1

CRN 2398-70-1
CMF C7 H8 N4 O S



CM 2

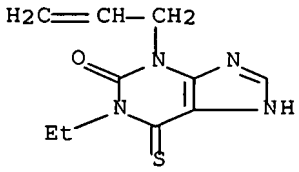
CRN 62-49-7
CMF C5 H14 N O



RN 879632-11-8 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1-ethyl-1,3,6,7-tetrahydro-3-(2-propenyl)-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

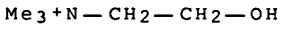
CM 1

CRN 42459-02-9
CMF C10 H12 N4 O S



CM 2

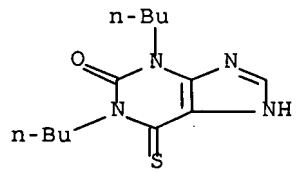
CRN 62-49-7
CMF C5 H14 N O



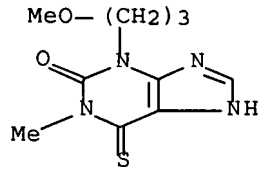
IT **40915-18-2**, Xanthine, 1,3-dibutyl-6-thio- **42458-94-6**,

Xanthine, 3-(3-methoxypropyl)-1-methyl-6-thio- **42458-99-1**, Xanthine, 3-furfuryl-1-methyl-6-thio- **42459-02-9**, Xanthine, 3-allyl-1-ethyl-6-thio- **42459-04-1**, Xanthine, 1-ethyl-3-isobutyl-6-thio- **93263-24-2**, Xanthine, 3-isobutyl-6-thio-
(sodium derivative, blood-vessel and bronchial dilation by)

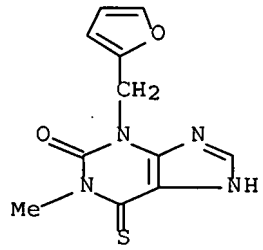
RN 40915-18-2 CAPLUS
CN 2H-Purin-2-one, 1,3-dibutyl-1,3,6,7-tetrahydro-6-thioxo- (9CI) (CA INDEX NAME)



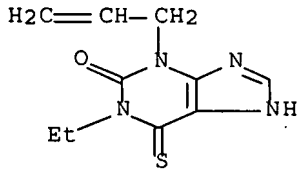
RN 42458-94-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-(3-methoxypropyl)-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



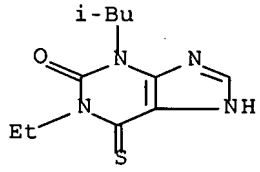
RN 42458-99-1 CAPLUS
CN 2H-Purin-2-one, 3-(2-furanylmethyl)-1,3,6,7-tetrahydro-1-methyl-6-thioxo- (9CI) (CA INDEX NAME)



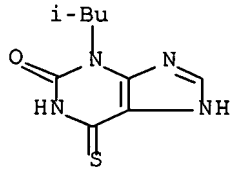
RN 42459-02-9 CAPLUS
CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-(2-propenyl)-6-thioxo- (9CI) (CA INDEX NAME)



RN 42459-04-1 CAPLUS
CN 2H-Purin-2-one, 1-ethyl-1,3,6,7-tetrahydro-3-(2-methylpropyl)-6-thioxo- (9CI) (CA INDEX NAME)



RN 93263-24-2 CAPLUS
CN Xanthine, 3-isobutyl-6-thio- (7CI) (CA INDEX NAME)



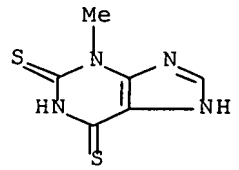
L57 ANSWER 107 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:38398 CAPLUS Full-text
DOCUMENT NUMBER: 56:38398
ORIGINAL REFERENCE NO.: 56:7262f-i,7263a-c
TITLE: Preparation and peracid oxidation of 2-(p-dimethylamino)styrylpyridine
AUTHOR(S): Pentimalli, L.
CORPORATE SOURCE: Univ. Bologna, Italy
SOURCE: Tetrahedron (1961), 14, 151-60
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB cf. CA 54, 21087a. -In substituted pyridines electronic interaction between an electron-donor substituent and the pyridine nucleus is greatest when the substituent is bonded directly to the nucleus, but is decreased when the bonding takes place through a system of double bonds. It was shown that interaction effects between the NMe2 group and the pyridine ring in the title compound, 2-(p-Me2NC6H4CH:CH)C5H4N (I) are small. KOH (1.0 g.), 2.2 g. 2-MeC5H4NO, and 4.3 g. p-Me2NC6H4CHO refluxed gently 6 hrs. in 6 ml. anhydrous C5H5N, the cooled mixture stirred 20 min. in 100 ml. cold H2O, the H2O-washed

and dried precipitate shaken with 30 ml. cold Me2CO and filtered yielded 57% bright yellow II, m. 200-1°, showing the bathochromic shift of conjugated substituted pyridine 1-oxides. II (4 g.) in 80 ml. AcOH at 90° stirred 20 min. with gradual addition of 6 g. Fe powder at 100°, the mixture kept 15 min. and the cooled mixture made strongly alkaline by addition of dilute NaOH, the washed and dried powdered product extracted twice with 50 ml. boiling C6H6 and the residue on evaporation (m. 136-8°) recrystd. from MeOH yielded 60% I, m. 139°. In strongly acidic medium both pyridine and amine N atoms undergo protonation, impeding the conjugative interaction with consequent decrease of absorption. I (1.0 g.) in 8 ml. CHCl3 at 15° slowly treated with 0.7 g. BzO2H in CHCl3, the mixture kept 16 hrs. and shaken with saturated aqueous Na2CO3, the dried solution (anhydrous Na2CO3) filtered and the solvent evaporated gave colorless plates of 2-[p-Me2N(O)C6H4CH:CH]C5H4N, m. 100° (decomposition) (C6H6). I (1.0 g.) in 10 ml. CHCl3 at 15° treated slowly with 1.7 g. BzO2H in CHCl3, kept 16 hrs., and the product isolated gave 2-[p-Me2N(O)C6H4CH: CH] C5H4NO, m. 148° (C5H5N), also obtained by oxidation of 4 g. II in 40 ml. CHCl3 with 2.76 g. BzO2H in CHCl3. Condensation of 4.7 g. α-MeC5H4N with 4.6 g. BzH in 2.9 ml. AcOH containing 4.8 ml. Ac2O gave 2(PhCH:CH)C5H4N, m. 89-90°. The corresponding 2(PhCH:CH)C5H4NO was obtained by condensation of 2.2 g. 2-MeC5H4NO with 3 g. BzH with KOMe in 5 ml. MeOH to give material, m. 162-3° (C6H6), also prepared by oxidation of 7.2 g. base with 6.3 ml. 36% H2O2 in 25.7 ml. AcOH. It was concluded that the 1st O atom in the stepwise oxidation of I is bonded only to the amino N atom and the 2nd to the pyridine ring N atom. As with the corresponding azo derivative, the electron d. remained highest at the NH2 N atom in comparison with the d. at the pyridine N atom.

IT **33285-77-7P**, Xanthine, 3-methyl-2,6-dithio-
RL: PREP (Preparation)
(preparation of)

RN 33285-77-7 CAPLUS

CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L57 ANSWER 108 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1962:25096 CAPLUS Full-text

DOCUMENT NUMBER: 56:25096

ORIGINAL REFERENCE NO.: 56:4762b-h

TITLE: Synthesis and properties of 3-methylpurines

AUTHOR(S): Bergmann, Felix; Levin, Gershon; Kalmus, Abraham; Kwietny, Hanna

CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem, Israel

SOURCE: Journal of Organic Chemistry (1961), 26, 1504-8
CODEN: JOCEAH; ISSN: 0022-3263

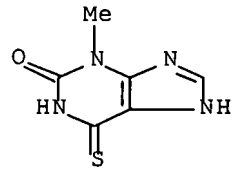
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

AB A series of substituted purines was prepared and, by comparison of their ultraviolet spectra, it was deduced that 3-methylhypoxanthine (I), 8-hydroxy-3-methyl-6-purinone (II), 3-methyl-8 hydroxypurine (III), 3-methylpurine-6-

RN 33285-76-6 CAPLUS
CN 2H-Purin-2-one, 1,3,6,7-tetrahydro-3-methyl-6-thioxo- (9CI) (CA INDEX NAME)

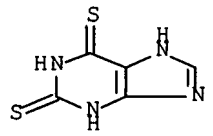


L57 ANSWER 109 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:18329 CAPLUS Full-text
DOCUMENT NUMBER: 56:18329
ORIGINAL REFERENCE NO.: 56:3480c-i,3481a-b
TITLE: Synthesis of 8-substituted purines
AUTHOR(S): Bergmann, F.; Tamari, M.
CORPORATE SOURCE: Hebrew Univ., Jerusalem, Israel
SOURCE: Journal of the Chemical Society (1961) 4468-72
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 56:18329
ED Entered STN: 22 Apr 2001
AB Condensation of an acetamidine salt with an appropriate derivative of 4,5-diaminopyrimidine in the absence of a solvent led directly to high yields of the 8-substituted purines (I). General procedure. A mixture of a 4,5diaminopyrimidine and 2 equivs. MeC(:NH)NH2.HCl (II.HCl) heated to 180-90° (homogeneous melt was formed and NH3 was evolved), when reaction ceased, the melt dissolved in N NaOH, the solution decolorized with C, and acidified with AcOH to pH 6 gave the I, all decomposing above 310° [substituents at 2-, 6-, and 8-position, reaction time in min., % yield, λ (mμ) at pH 8.0, Rf in 85:10:5 95% EtOH-H2OAcOH (solvent A), 70:20:10 95% EtOH-pyridine-H2O (solvent B), and 65:25:10 iso-PrOH-HCONMe2-10% aqueous NH3 (solvent C) given]: H, OH, Me, 60, 56 (the yield was improved by addition of 2 equivs. anhydrous NaOAc), 2.52, 0.57, 0.70, --; H, OH, Me, 60, 67 (with II.AcOH), --, --, --, --; OH, OH, Me, 30, 94, 240 and 275, 0.54, 0.60, 0.42; OH, SH, Me (III), 35, 83 (the yield was improved by addition of 2 equivs. anhydrous NaOAc) (the same compound was also prepared in 90% yield from 8-methylxanthine with P2S5), 251 and 344, 0.50, 0.56, 0.57; SH, OH, Me, 30, 77, 235 and 280, 0.45, 0.74, 0.61; SH, SH, Me, 25, 65 (the yield was improved with 2 equivs. anhydrous NaOAc), 247 and 285, and 351, 0.53, 0.59, 0.71; SH, SH, Me (IV), 25, 86 (with II.AcOH), --, --, --, --; SH, NH2, Me (V), 30, 66 (isolated as the sulfate), 230 and 251, and 280, 0.61, 0.67, --; H, OH, Ph, 70, 50, 291, 0.58, 0.79, --; H, OH, Ph, 70, 78 (with II.AcOH), --, --, --; OH, OH, Ph, 40, 80, 228 and 309, 0.52, 0.66, --. Also were prepared 92% 3,8-dimethylxanthine (VI), λ (pH 8.0) 275 m, Rf 0.64 (in A), 0.79 (in B), and 0.68 (in C), and 88% 3,8-dimethyl-2-mercaptoxanthine (VII), λ (pH 8.0), 233 and 288 mμ, Rf 0.60 (in A) and 0.84 (in B). N:C(OH).-N:C(NH2).C(NH2):CH (VIII) (Kalmus and Bergmann, CA 55, 12418h) (1 g.), 1 g. II.HCl, and 0.8 g. anhydrous NaOAc heated 20 min. at 140-5, the resulting cake dissolved in 10% aqueous NH3, the solution boiled with C, filtered, and the filtrate kept 24 hrs. in a cold room gave 0.65 g.

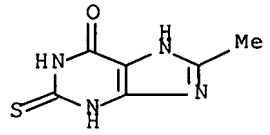
inseparable mixture of VIII and 2-hydroxy-8-methylpurine (IX), (pH 8.0) 307 m. III (5 g.) and 1.5 g. (wet weight) Raney Ni in 25 ml. 5% aqueous NH3 refluxed 80 min., filtered, the filtrate adjusted to pH 2 with HNO3, and kept 2 months at room temperature gave IX.HNO3. If the above ammoniacal solution was acidified with H2SO4, IX decomposed quant. The same result was obtained when an ammoniacal solution of IX was evaporated to dryness, the residue extracted with absolute EtOH, and the mixture acidified with 1% alc.-H2SO4. V (580 mg.) and 1.5 g. (wet weight) Raney Ni in 100 ml. 5% aqueous NH2 refluxed 2 hrs., filtered hot, and the filtrate cooled gave 300 mg. 8-methyladenine, Rf 0.57 (in A), 0.67 (in B), and 0.64 (in C). 8-Methylhypoxanthine (1.3 g.), 5 g. P2S5, and 50 ml. dry pyridine refluxed 4 hrs., concentrated in vacuo, the residue extracted with 37 NaOH, filtered, the solution concentrated in vacuo, and kept overnight at 0° gave 1.1 g. 6-mercapto-8-methylpurine, decomposed above 310° (H2O), (pH 8.0) 232 and 316 m, Rf 0.64 (in A) and 0.71 (in C). VII (1 g.) and 0.7 ml. MeI stirred 30 min. at room temperature in 10 ml. 0.5N NaOH gave 0.95 g. 3,8-dimethyl2-(methylthio)hypoxanthine, decomposed at 312-15° (H2O), Rf 0.73 (in B). VII (2 g.) and 6 g. (wet weight) Raney Ni in 50 ml. 5% aqueous NH3 refluxed 2 hrs., filtered, and concentrated in vacuo gave 1.4 g. 3,8-dimethylhypoxanthine, decomposed at 300° (EtOH), Rf 0.6 (in B). NH.CO.NMe.C(NH2):C- (NH2).CS (X) and II.HCl or II.AcOH heated at 150-200° gave only X and tars. VI treated with P2S5 in pyridine, concentrated in vacuo, the residue decomposed with cold dilute aqueous NH3, the mixture filtered, and the filtrate adjusted to pH 6 with AcOH gave only X, λ (pH 8.0) 249 and 344 mμ, Rf 0.33 (in A). IV (1 g.) and 2.5 g. Raney Ni in 50 ml. 5% aqueous NH3 refluxed 70 min., filtered, the filtrate concentrated in vacuo, and kept overnight gave 150 mg. 8-methylpurine, λ (pH 8.0) 266 mμ, Rf 0.75 (in A).

IT **5437-25-2P**, Xanthine, dithio- **91184-09-7P**, Xanthine, 8-methyl-2-thio- **91184-10-0P**, Xanthine, 8-methyl-6-thio- **91725-06-3P**, Xanthine, 3,8-dimethyl-2-thio-
RL: PREP (Preparation)
(preparation of)

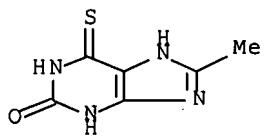
RN 5437-25-2 CAPLUS
CN 1H-Purine-2,6-dithione, 3,9-dihydro- (CA INDEX NAME)



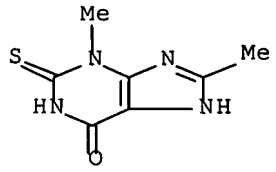
RN 91184-09-7 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 91184-10-0 CAPLUS
CN Xanthine, 8-methyl-6-thio- (7CI) (CA INDEX NAME)



RN 91725-06-3 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3,8-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)



L57 ANSWER 110 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:60865 CAPLUS Full-text
DOCUMENT NUMBER: 55:60865
ORIGINAL REFERENCE NO.: 55:11652a-d
TITLE: Thioxanthines with potent bronchodilator and coronary dilator properties
AUTHOR(S): Armitage, A. K.; Boswood, Janet; Large, B. J.
CORPORATE SOURCE: May and Baker, Dagenham, UK
SOURCE: British Journal of Pharmacology and Chemotherapy (1961), 16, 59-76
CODEN: BJPCAL; ISSN: 0366-0826
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB The pharmacol. properties of 2 new compds., choline 6-thiotheophyllinate (I) and the choline salt of 3-isobutyl-1-methyl-6-thioxanthine (M & B, 5924) (II) are described. As bronchodilators on the isolated guinea pig tracheal ring preparation, I and II were 57 and 5 times, resp., more active than choline theophyllinate (III). In protective effect against bronchioconstrictor aerosols, III (50 and 100 mg./kg., i.p.) was almost identical with that of I. II (100 mg./kg. orally) appeared to give more protection than III (200 mg./kg.). I and II had very little antihistaminic and antiacetylcholine activity. In cardiovascular studies on the anesthetized cats and dogs, all 3 compds. caused a transient fall in blood pressure. I and II were more potent than III as coronary dilators on the dog heart-lung preparation As diuretics they were less potent. In doses up to 20 mg./kg., III increased the voluntary locomotor activity of mice. A 50% increase was produced by 12 mg. of I and II each/kg. However, other doses from 5 to 80 mg./kg. either decreased motor activity or had no effect. A 50% decrease in motor activity was produced by 32 mg. I/kg. and by 30 mg. II/kg. Toxic doses of III caused intense excitement and convulsions, whereas toxic doses of the thioxanthines caused sedation. Death in all cases was due to respiratory failure. In dogs, I in doses as high as 120 mg./kg., orally, caused no ill effects; II at 60 and 80 mg./kg. caused vomiting and retching lasting for about 1 h. II given i.v. to

dogs in doses up to 3 mg./kg. caused vomiting, retching, excitation, and restlessness in contrast to the sedation seen in mice.

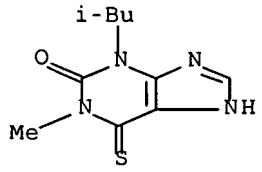
IT **857018-10-1**, Xanthine, 3-isobutyl-1-methyl-6-thio-, compound with choline **878794-41-3**, Theophylline, 6-thio-, compound with choline
(pharmacol. of)

RN 857018-10-1 CAPLUS

CN Xanthine, 3-isobutyl-1-methyl-6-thio-, compd. with choline (6CI) (CA INDEX NAME)

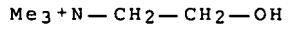
CM 1

CRN 42458-91-3
CMF C10 H14 N4 O S



CM 2

CRN 62-49-7
CMF C5 H14 N O

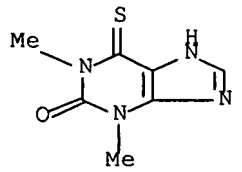


RN 878794-41-3 CAPLUS

CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 2398-70-1
CMF C7 H8 N4 O S

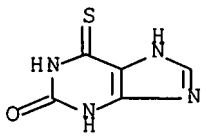


CM 2

CRN 62-49-7
CMF C5 H14 N O

$Me_3{}^+N-CH_2-CH_2-OH$

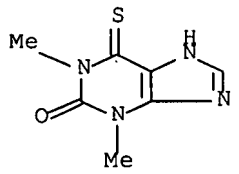
L57 ANSWER 111 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:56289 CAPLUS Full-text
DOCUMENT NUMBER: 55:56289
ORIGINAL REFERENCE NO.: 55:10804b-d
TITLE: 1,3-Dialkyl-6-thioxanthines: a new series of bronchodilators and coronary vasodilators
AUTHOR(S): Armitage, A. K.; Wooldridge, K. R. H.
CORPORATE SOURCE: May & Baker, Ltd., Dagenham, UK
SOURCE: Nature (London, United Kingdom) (1960), 188, 1107-8
CODEN: NATUAS; ISSN: 0028-0836
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB Thioxanthines were prepared from the corresponding xanthines by refluxing for several hrs. with P2S5 in pyridine. Thionation occurred in the 6-position only. The choline salt of 3-isobutyl-1-methyl-6-thioxanthine (I), the most active derivative in vitro for relaxation of the bronchial muscle and dilation of the coronary vessels, is pale-yellow, crystalline, solid, m. 145-7°, and >50% soluble in H2O at 20°. Choline 6-thiotheophyllinate (II), m. 146-9°, has similar solubility The thio derivs. are more active in vitro than in vivo. I is more active than II in dilating the coronary vessels of the dog heart-lung preparation or of the anesthetized dog, and in dilating the vessels of the hind leg of the dog perfused with heparinized blood.
IT **2002-59-7**, Xanthine, 6-thio-
(1,3-dialkyl derivs., as bronchodilators and coronary vasodilators)
RN 2002-59-7 CAPLUS
CN 2H-Purin-2-one, 1,3,6,9-tetrahydro-6-thioxo- (CA INDEX NAME)



IT **878794-41-3**, Theophylline, 6-thio-, compound with choline
(as bronchodilator and coronary vasodilator)
RN 878794-41-3 CAPLUS
CN Ethanaminium, 2-hydroxy-N,N,N-trimethyl-, compd. with 1,3,6,7-tetrahydro-1,3-dimethyl-6-thioxo-2H-purin-2-one (1:1) (9CI) (CA INDEX NAME)

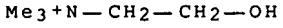
CM 1

CRN 2398-70-1
CMF C7 H8 N4 O S



CM 2

CRN 62-49-7
CMF C5 H14 N O



L57 ANSWER 112 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:39968 CAPLUS Full-text
DOCUMENT NUMBER: 53:39968
ORIGINAL REFERENCE NO.: 53:7191g-i,7192a-i
TITLE: Potential purine antagonists. XIII. Synthesis of some 8-methylpurines
AUTHOR(S): Koppel, Henry C.; Robins, Rolland K.
CORPORATE SOURCE: Arizona State Coll., Tempe
SOURCE: Journal of Organic Chemistry (1958), 23, 1457-60
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 53:39968
ED Entered STN: 22 Apr 2001
AB cf. C.A. 53, 1366a. Use of Ac2O as a general cyclizing agent for 4,5-diaminopyrimidines was investigated. A number of new 8-methylpurines were prepared 4,5-Diamino-6-hydroxypyrimidine (I) with Ac2O gave 70% 6-hydroxy-8-methylpurine (II). I (15 g.) refluxed 80 min. in 250 ml. Ac2O, excess Ac2O removed in vacuo, the sirupy residue refluxed 10 min. in 250 ml. 1.5N NaOH, treated with C, cooled, acidified, and separated gave 14 g. II.H2O, m. above 300°. II (35 g.) added to 500 ml. POCl3 and 50 ml. PhNMe2, the mixture refluxed 5.5 hrs., excess POCl3 removed, the residue poured on ice, made strongly basic, left 20 min., extracted with Et2O, the solution acidified, continuously extracted with Et2O, and concentrated gave 18 g. 6-chloro-8-methylpurine (III), m. 212-13° (PhMe). III (5 g.) refluxed 1 hr. with 150 ml. alc. containing 10 g. CS(NH2)2, chilled, filtered, the product refluxed with 150 ml. dilute NaOH, and acidified gave 3.9 g. 8-methyl-6-purinethiol (IV), m. above 300°(H2O). IV (5 g.) refluxed 6 hrs. with 100 ml. H2O containing 15 g. Raney Ni, the Ni removed, washed with 50 ml. boiling H2O, the combined filtrate and washings evaporated to dryness, and crystallized gave 3.2 g. 8-methylpurine (C6H6-heptane-MeOH). III (5 g.) heated 2 hrs. with 50 ml. H2O containing 50 ml. 40% MeNH2 gave 3.8 g. 6-methylamino-8-methylpurine, m. above 300° (H2O). III (5 g.) heated 2 hrs. with 150 ml. alc. and 9 g. p-ClC6H4CH2NH2 gave 4.2 g. 8-methyl-6-(p-chlorobenzylamino)purine, m. above 300°(alc.). III (5 g.) heated 3 hrs. with 150 ml. alc. and 10 g. 2,4-Cl2C6H3CH2NH2 gave 4 g. 6-(2,4-dichlorobenzylamino)-8-methylpurine, m. 286-7° (alc.). IV (5 g.) in 100 ml. hot H2O containing 5 g. KOH treated 3 hrs. with 4

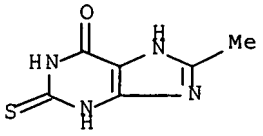
g. MeI, the pH adjusted to 7, and cooled gave 3 g. 6-methylthio-8-methylpurine, m. 223-4°(C6H6heptane-MeOH). The following 6-alkylthio-8-methylpurines were prepared by a general method as shown below. IV (5 g.) heated 0.5 hr. with 75 ml. H2O, 3 g. KOH, and 10 g. EtSH, the pH adjusted to 7 with dilute HCl, and the crude product collected gave 3.6 g. 6-ethylthio-8-methylpurine (V), m. 206-7°(EtOAc-heptane). The following 6-alkylthio analogs of V were similarly prepared (alkyl given): Pr, m. 214-15° (C6H6-heptane); iso-Pr, m. 256-7° (EtOAc-heptane); Bu, m. 179-80° (C6H6-heptane-MeOH). 4,5-Diamino-6-hydroxy-2-mercaptopyrimidine (10 g.) refluxed 9 hrs. in 250 ml. Ac2O, cooled, the solid collected, washed, refluxed 10 min. with 250 ml. 1.5N NaOH, and acidified gave 11.5 g. 6-hydroxy-8-methyl-2-purinethiol (VI), m. above 300° (dilute AcOH). VI (20 g.) in 500 ml. 0.5N NaOH stirred with 15 g. MeI until only one phase resulted, the solution heated to 80° treated with C, acidified, and cooled gave 14 g. 6-hydroxy-8-methyl-2-methylthiopurine (VII), m. above 300°(H2O). 4,5-Diamino-6-hydroxy-2-(methylthio)pyrimidine (23 g.) refluxed 2 hrs. in 250 ml. Ac2O, excess Ac2O distilled, the residue refluxed in 250 ml. 1.5N NaOH, the solution acidified, and cooled gave 22 g. VII, identical with the above prepared specimen. VI (15 g.) refluxed 5 hrs. in 500 ml. C5H5N containing 60 g. P2S5, the excess C5H5N removed, 300 ml. H2O added, the mixture heated 3 hrs., cooled, the product collected, and repptd. twice from dilute Na2CO3 with acid gave 8-methyl-2,6-purinedithiol, m. above 300°. VII (35 g.) refluxed 3.5 hrs. with 500 ml. POCl3 and 70 ml. PhNEt2, excess POCl3 removed in vacuo, the residue poured on ice, made basic, extracted with Et2O, the aqueous solution kept at 10°, acidified to pH 1, left 3 hrs., and the solid collected gave 21 g. 6-chloro-8-methyl-2-(methylthio)purine (VIII), m. 268-70°(PhMe). VIII (5 g.) refluxed 1 hr., cooled, the crude product dissolved in dilute KOH, and repptd. with AcOH gave 4.1 g. 8-methyl-2-methylthio-6-purinethiol (IX), m. above 300° (dilute AcOH). IX (5 g.) in 150 ml. alc. heated with 10 g. p-ClC6H4CH2NH2 until the volume reached 75 ml. and cooled gave 5.4 g. 6-(p-chlorobenzylamino)-8- methyl-2-(methylthio)purine, m. 265-6° (alc.). VIII (5 g.) in 100 ml. alc. heated with 10 g. Me2NNH2 until the volume was reduced to half and cooled gave 3.9 g. 6-(unsym-dimethylhydrazino)-8-methyl-2- (methylthio)purine, needles, m. 289-91°(alc.). VIII (5 g.), 125 ml. alc., and 10 g. NHEt2 similarly heated and evaporated gave 2.8 g. 6-diethylamino-8-methyl-2-(methylthio)purine, m. 216-18° (heptane-alc.). VIII (5 g.), 100 ml. 40% MeNH2, and 50 ml. H2O similarly treated gave 4 g. 8-methyl-6-methylamino-2-(methylthio)purine, m. 209° (alc.). 6-Dimethylamino-8-methyl-2-(methylthio)purine was similarly prepared 4,5,6-Triaminopyrimidine (15 g.) refluxed 2 hrs. with 150 ml. Ac2O, excess Ac2O removed, the residue dissolved in 300 ml. refluxing dilute NH4OH, the cooled solution filtered, the solid purified, and repptd. gave 12 g. 6-amino-8-methylpurine, m. above 300°(HCONMe2). 2,4,5-Triamino-6-hydroxypyrimidine (22 g.) refluxed 5 hrs. with 500 ml. 1:1 Ac2O-HC(OEt)3, distilled, the sirupy residue refluxed 10 min. in 250 ml. 2N NaOH, and acidified gave 12 g. 2-amino-6-hydroxy-8-methylpurine, m. above 300°. 2,6-Dihydroxy-4,5-diaminopyrimidine (10 g.) refluxed 12 hrs. in 250 ml. Ac2O and the crude product refluxed in 250 ml. 2N NaOH gave 10 g. 2,6-dihydroxy-8-methylpurine, m. above 300°. 4,5-Diamino-6-pyrimidinethiol (2.5 g.) refluxed 3 hrs. with 50 ml. Ac2O and the sirupy residue refluxed 10 min. in 100 ml. dilute NH4OH gave 2 g. 7-amino-2-methylthiazolo[5,4-d]pyrimidine. A general H2O-solubilizing effect of the 8-Me group as compared to the corresponding simple purine derivative was noted. This group may interfere with the intermol. H bonding forces in the crystal lattice. This effect is not noted in the parent compound, 8-methylpurine. The ultraviolet absorption of some β-methylpurines are recorded.

IT **91184-09-7P**, Xanthine, 8-methyl-2-thio- **91184-18-8P**, Xanthine, 8-methyldithio-
RL: PREP (Preparation)
(preparation of)

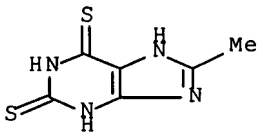
RN 91184-09-7 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-8-methyl-2-thioxo- (9CI) (CA INDEX

NAME)



RN 91184-18-8 CAPLUS
CN Xanthine, 8-methyl-2,6-dithio- (7CI) (CA INDEX NAME)

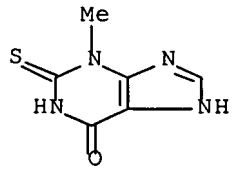


L57 ANSWER 113 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1959:34829 CAPLUS Full-text
DOCUMENT NUMBER: 53:34829
ORIGINAL REFERENCE NO.: 53:6243f-i,6244a-c
TITLE: Some new N-methylpurines
AUTHOR(S): Elion, Gertrude B.
CORPORATE SOURCE: Wellcome Research Labs., Tuckahoe, NY
SOURCE: Ciba Foundation Symposium, Chem. and Biol. Purines (1957) 39-49
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB Ring closure in 5-formamido-4-amino-3-methyl-2-mercapto-6-oxopyrimidine (I) gave 2-mercapto-3-methylhypoxanthine (II), which on treatment with Raney Ni provided 3-methylhypoxanthine (III). I with Raney Ni gave 5-formamido-4-amino-3-methyl-6-oxopyrimidine which underwent ring closure with formamide to form III. III with P2S5 in pyridine provided 3-methyl-6-mercaptopurine which when treated with NH4OH at 140° for 16 h. gave 3-methyladenine (IV). Excellent yields of IV were obtained by treatment of II with P2S5 to form 3-methyl-2,6-dithiopurine, which was then converted to the 6-amino derivative and treated with Raney Ni to give IV. Methylation of 5-formamido-4-amino-2-mercapto-6-oxopyrimidine (V) with Me2SO4 in aqueous alkali gave the 2-methylthio-1-Me derivative (VI), as well as a water-soluble compound believed to be 4-amino-5-formamido-2-methylthio-6- methoxypyrimidine. VI with Raney Ni gave 5-formamido-4-amino-1-methyl-6- oxopyrimidine, which was converted to 1-methylhypoxanthine (VII) by heating with HCO2H. Treatment of VII with P2S5 in Tetralin or pyridine gave 1-methyl-6-mercaptopurine (VIII). Cyclization of VI with HCO2H gave 2-methylthio-1-methylhypoxanthine, which yielded 1-methylxanthine on acid hydrolysis and 1-methylguanine on heating with NH4OH. Heating of VIII with aqueous NH3 at 140° gave 4-amino-5-imidazolecarboxamide. With alc. NH3 at 160°, VIII was converted to 6-(methylamino)purine. VI with P2S5 in pyridine gave 2-methylthio-1-methyl-6-thiopurine, which when heated with NH4OH at 140° formed 1-methyl-2,6-diaminopurine. When 6-chloropurine was methylated and then treated with NaSH, 7-methyl- and 9-methyl-6-mercaptopurines were formed. These were easily separated because of a

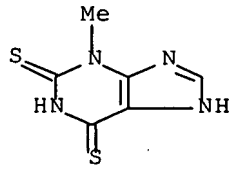
difference in solubility in water. 9-Methyladenine, prepared from 6-amino-2-methylthio-9-methylpurine, gave 9-methylhypoxanthine on treatment with HNO2. The UV absorption maximum (in mμ) at pH 1, 3, 7, and 11 were, for substituted hypoxanthines were (substituent given): H, 248, -, 249, 258; 1-Me, 249, -, 251, 260; 3-Me, 253, 262, 264, 265; 7-Me, 250, 255, 256, 262; 9-Me, 250, -, 250, 254. For substituted purines: 6-MeO, 254, -, 252, 261; 6-HS, 325, 323, 322, 233 (312); 1,6-Me(HS), 229(321), 233(321), 235(320), 237(321); 3,6-Me(HS), 244(334), 245(340), 245(337), 245(332); 7,6-Me(HS), 328, 328, 327, 234(315); 9,6-Me(HS), 323, 321, 320, 234(309); 6-MeS, 294, 290, 290, 290. At pH 1 and 11 for substituted adenines: H, 263, 267; 3-Me, 274, 273; 7-Me, 272, 271; 9-Me, 261, 262. 6-Methylaminopurine: 267, 272, at pH 1 and 11.

IT **28139-02-8P**, Xanthine, 3-methyl-2-thio- **33285-77-7P**, Xanthine, 3-methyldithio-
RL: PREP (Preparation)
(preparation of)

RN 28139-02-8 CAPLUS
CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)



RN 33285-77-7 CAPLUS
CN 1H-Purine-2,6-dithione, 3,7-dihydro-3-methyl- (9CI) (CA INDEX NAME)



L57 ANSWER 114 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1954:11249 CAPLUS
DOCUMENT NUMBER: 48:11249
ORIGINAL REFERENCE NO.: 48:2093a-e
TITLE: Substituted imidazoles and xanthines
INVENTOR(S): Heilbron, Ian M.; Cook, Arthur H.
PATENT ASSIGNEE(S): Beecham Research Laboratories Ltd.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 683523		19521203	GB 1948-21834	19480818 <--

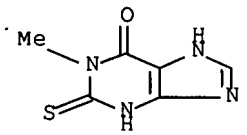
ED Entered STN: 22 Apr 2001

AB NH2CH(CN)CO2Et and HC(:NH)NH2.HCl refluxed 2 h. in 10:1 CHCl3-EtOH give 40% Et 4-amino-5-imidazolecarboxylate (I), m. 180-1°. I and MeNCS refluxed 1 h. in C5H5N and the solution poured into H2O gives the 4-(3-methyl-2-thioureido) analog (II) of I, m. 163°. II dissolved in 2N NaOH solution and the solution acidified with AcOH gives 1-methyl-2-thioxanthine, also prepared in 62% yield by this reaction series without isolating the intermediates. Similarly are prepared these xanthines: 1,8-di-Me, 8-Ph, 1-methyl-8-Ph (m. above 360°), 7-methyl-8-Ph [m. 340° (decomposition)], 8-benzyl-1-Ph [m. 318° (deeompn.)], 1-methyl-8-(p-nitrobenzyl), 1,8-dimethyl-2-thio, 8-phenyl-2-thio (decompose above 360°), 1-methyl-8-phenyl-2-thio, 8-benzyl-1-phenyl-2-thio (m. above 360°), 8-benzyl-1,7-dimethyl-2- thio, m. above 360°, and 1,7-dimethyl-8-phenyl-2-thio, m. above 360°. This patent also includes all the intermediates of the following 2 patents. Brit. 683,593 and 683,594 cover the intermediates of types II and I, resp., of the preceding patent. The following substituted Et 5-imidazolecarboxylates were also prepared (substituents and m.ps. given): 4-amino-2-Me, 167° (decomposition) [HCl salt, m. 213-14° (decomposition)]; 4-amino-2-Ph HCl salt, 216°; 4-amino-2-benzyl HCl salt, 196° (decomposition); 4-amino-2-(p-nitrobenzyl) HCl salt, 226°, 4-amino-2-benzyl-1-Me, 145°; 4-amino-1-methyl-2-Ph, 140-2°; 2-phenyl-4-ureido, 193-5°; 2-phenyl-4-thioureido, 255°; 4-(3-acetyl-2-thioureido)-2-Ph, 225°; 1-methyl-2-phenyl-4-ureido, 193-4°; 2-methyl-4-(3-methyl-2- thioureido), 194°; 4-(3-methylureido)-2-Ph, 181-2°; 4-(3-methyl-2-thioureido)-2-Ph, 245°; 2-benzyl-4-(3-phenylureido), 187°; 2-benzyl-4-(3-phenyl-2-thioureido), 195°; 2-benzyl-1-methyl-4-(3-methyl-2-thioureido), 191°; 1-methyl-4-(3-methyl-2-thioureido)-2-Ph, 185-9°; and 4-(3-methylureido)-2-(p-nitrobenzyl), 242° (decomposition). Cf. Cook, C.A. 45, 1034bf.

IT **91184-08-6P**, Xanthine, 1-methyl-2-thio- **874519-01-4P**, Xanthine, 1,8-dimethyl-2-thio-
RL: PREP (Preparation)
(preparation of)

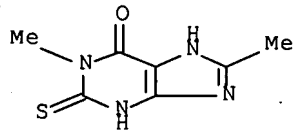
RN 91184-08-6 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-2-thioxo- (9CI) (CA INDEX NAME)



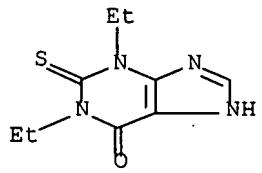
RN 874519-01-4 CAPLUS

CN Xanthine, 1,8-dimethyl-2-thio- (5CI) (CA INDEX NAME)



L57 ANSWER 115 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1951:61193 CAPLUS Full-text
DOCUMENT NUMBER: 45:61193

ORIGINAL REFERENCE NO.: 45:10401e-g
TITLE: Diuretic activity of compounds related to xanthines, uracils, and triazines as determined in dogs
AUTHOR(S): Kattus, Albert A.; Newman, Elliot V.; Franklin, John
CORPORATE SOURCE: Johns Hopkins Univ., Baltimore, MD
SOURCE: Bulletin of the Johns Hopkins Hospital (**1951**), 89, 1-8
CODEN: JHHBAI; ISSN: 0097-1383
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
AB A series of 19 substituted xanthines, 1 thioxanthine, 14 uracils, 1 thiouracil, 3 triazines, 2 phenothiazines, and a substituted N-benzylaniline were tested for diuretic activity in female dogs. Urine vols. and Na excretions from dogs receiving two 0.25-0.5-g. doses in 1 day were compared with those from the same dogs prior to dosing. With Na excretion as a criterion, 1,3-diethylxanthine (I), its 2-thio analog, and its 8-bromo derivative (II) were highly diuretic, but caused emesis. Emesis was also noted with other 1,3-dialkylxanthines. In human subjects I caused diuresis and vomiting, but II had neither action. Except for 1-propyl-3-ethyl-6-aminouracil, uracil derivs. were less active than the xanthine derivs. and produced less gastrointestinal disturbance; 2,4-bis(acetamido)-s-triazine produced diuresis in a human volunteer.
IT **841313-23-3**, Xanthine, 1,3-diethyl-2-thio-
(diuretic activity of)
RN 841313-23-3 CAPLUS
CN Xanthine, 1,3-diethyl-2-thio- (5CI) (CA INDEX NAME)



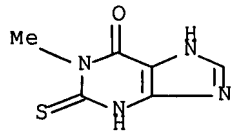
L57 ANSWER 116 OF 116 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1950:10067 CAPLUS Full-text
DOCUMENT NUMBER: 44:10067
ORIGINAL REFERENCE NO.: 44:1962a-i,1963a
TITLE: The azole series. XIV. A new synthesis of purines
AUTHOR(S): Cook, A. H.; Davis, A. C.; Heilbron, Ian; Thomas, G. H.
CORPORATE SOURCE: Imperial Coll. of Sci. and Technol., London
SOURCE: Journal of the Chemical Society (**1949**) 1071-4
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 44:10067
ED Entered STN: 22 Apr 2001
AB 4-Amino-5-carbethoxyglyoxalines and MeNCO or MeNCS gave the 4-(N-methylthioureido or ureido) compds., readily cyclized to 1-methylthioxanthines or xanthines. H2NCH2CO2Et (I) (15 g.), 30 g. PhCH2C(:NH)SCH2Ph.HCl (II), and 200 cc. dry CHCl3 were refluxed 1 h., concentrated to 90 cc., 100 cc. C6H6 added, and after 3 days at 0° the 20 g. HCl salt of 5-carbethoxy-2-benzyl-G (G

= 4-aminoglyoxaline) filtered, and 15 g. free base precipitated from hot H2O with NaOH; picrate, m. 221° (decomposition) (from EtOH). I (17 g.) and 15 g. PhC(:NH)OEt in 50 cc. Et2O 24 h. at room temperature gave 1.75 g. 5-carbethoxy-2-phenyl-G, m. 218° (decomposition) (from EtOH), and 0.4 g. more on concentration of the filtrate. The HCl salt, m. 216° (decomposition) (from MeOH), was obtained in 2.3-g. yield by 30 mins.' refluxing of 1.5 g. I, 3 g. PhC(:NH)SCH2Ph.HCl, and 25 cc. CHCl3; picrate, m. 224°; monoacetate, from Ac2O and H2SO4 and crystallized from H2O, m. 174°; 2-benzylideneamino compound, prepared in hot BzH and crystallized from EtOH, m. 214° (decomposition). 5-Carbethoxy-2-methyl-G, prepared in 0.1-g. yield from 2.5 g. I and 2.9 g. MeC(:NH)OEt 24 h. in Et2O at room temperature, m. 167° (decomposition) (from EtOH-Et2O); the HCl salt (65% from I and MeC(:NH)SCH2Ph.HCl refluxed 4 h. in CHCl3), m. 213-14° (decomposition), was easily converted to the free base. Addition of 5.6 g. HC(:NH)NH2.HCl with just sufficient EtOH for solution to 9 g. I in 200 cc. CHCl3, 2 h.' refluxing, 12 h.' standing of the blackened solution at room temperature, filtration from the 80% yield of NH4Cl, addition of Et2O to turbidity, filtration of a black oil after 6 h. at 0°, and concentration in vacuo gave 40% 5-carbethoxy-G, m. 180-1° (from EtOAc-EtOH). This product could not be prepared from HC(:NH)OEt or HC(:NH)OCHMe2. 5-Phenyl-2-benzyl-G, obtained in 45% yield by 12 h.' refluxing of 3 g. II and 1.7 g. PhCH(NH2)CN (III) in CHCl3, filtration of 3 g. HCl salt (m. 200° with decomposition), and liberation of the free base in the min. of warm H2O with NaOH, m. 199° (from MeOH); picrate, m. 215°; di-Ac derivative, m. 215° (from MeOH). PhC(:NH)SCH2Ph (2 g.) and 1 g. III similarly gave 1 g. 2,5-diphenyl-G, a white solid rapidly turning green; picrate, m. 220° (from EtOH). MeC(:NH)SCH2Ph.HCl (5 g.) and 3.5 g. III in boiling CHCl3 gave 5 g. crystalline product, very soluble in H2O and MeOH, insol. in Me2CO, and not diazotized in dilute HCl. It m. 125° on rapid heating, but 15 mins.' heating at 200° gave 5-phenyl-2-methyl-G.HCl, m. 238° (from MeOH), diazotizable in dilute HCl. Refluxing 1.2 g. 5-carbethoxy-2-benzyl-G 1 h. with 0.4 g. MeNCS in 5 cc. C5H5N, addition of H2O, and crystallization of the precipitate from EtOH gave 1.3 g. 5-carbethoxy-2-benzyl-MTG (MTG = 4-(3-methyl-2-thioureido)glyoxaline, m. 174°, converted by warming 1 min. in 10% NaOH and addition of excess HOAc to gelatinous 2-thio-8-benzyl-MX (MX = 1-methylxanthine). Similarly prepared, 5-carbethoxy-2-phenyl-MTG, m. 245°, converted by NaOH to 2-thio-8-phenyl-MX. 5-Carbethoxy-2-phenyl-G and MeNCO instead of MeNCS gave 5-carbethoxy-2-phenyl-MUG [MUG = 4-(3-methylureido)glyoxaline], m. 181-2°, converted by alkali to the corresponding 8-phenyl-MX; the latter was also formed by the action of H2O2 on 2-thio-8-phenyl-MX in 5% NaOH at 0° one week and then boiling and addition of excess HOAc. 5-Carbethoxy-2-methyl-MTG, prepared as above, m. 194° (from EtOAc), gave the 2-thio-8-methyl-MX. 5-Carbethoxy-2-methyl-G and MeNCO in C5H5N were refluxed 2 h., concentrated in vacuo, and the residue converted with alkali, etc., to 8-methyl-MX. 5-Carbethoxy-MTG, m. 163°, was converted to the 2-thio-MX. Addition of 0.5 g. KClO3 during 30 min. to 2 g. 8-phenyl-MX in 2.7 cc. concentrated HCl and 5 cc. H2O below 60° maintenance at 0° 1 h., filtration from the 0.6 g. precipitate, aeration for 3 h. to remove excess Cl, addition of 1.3 g. SnCl2 in 1 cc. concentrated HCl during 30 min. at 0 to -5°, and standing 12 h. at 0° gave 0.4 g. dimethylalloxantin, m. and mixed m.p. 200° (to a red liquid). This was converted by boiling with aqueous o-C6H4(NH3Cl)2 to 3-methylalloxazine, m. and mixed m.p. 280° (decomposition) (from HOAc-EtOH). 8-Methyl-MX similarly oxidized and reduced gave dimethylalloxantin, m. 207° (from H2O).

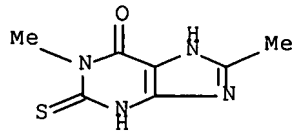
IT **91184-08-6P**, Xanthine, 1-methyl-2-thio- **874519-01-4P**, Xanthine, 1,8-dimethyl-2-thio-
RL: PREP (Preparation)
(preparation of)

RN 91184-08-6 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-1-methyl-2-thioxo- (9CI) (CA INDEX NAME)

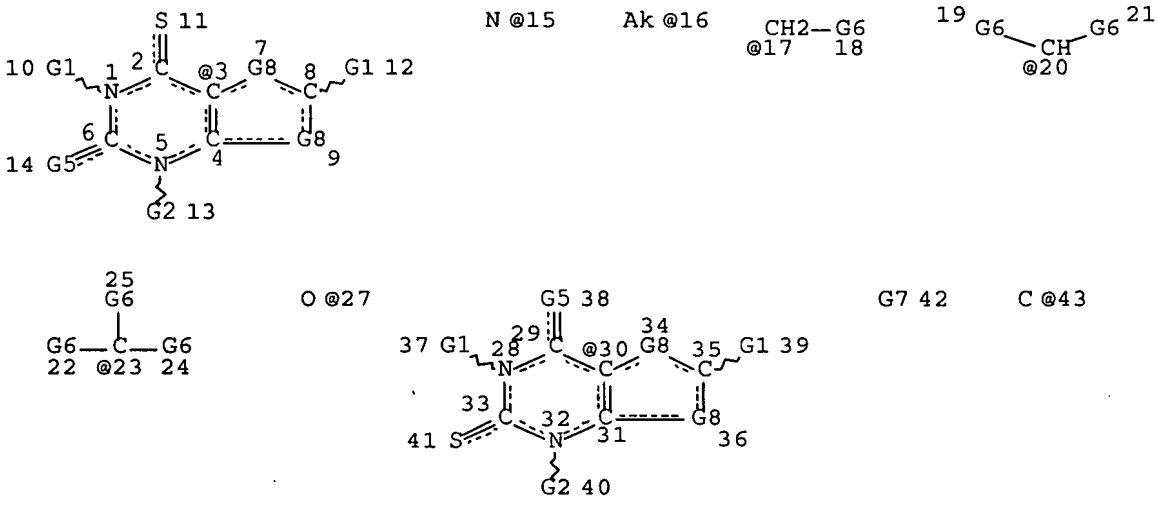


RN 874519-01-4 CAPLUS
CN Xanthine, 1,8-dimethyl-2-thio- (5CI) (CA INDEX NAME)



FILE 'HOME' ENTERED AT 15:03:12 ON 12 MAR 2007

```
=> d stat que l7; d his nofile
L4                STR
```




```
VAR G1=H/16
VAR G2=H/ME/17/20/23
VAR G5=O/S
VAR G6=27/43
VAR G7=3/30
VAR G8=15/NH/44
NODE ATTRIBUTES:
NSPEC    IS RC     AT  27
NSPEC    IS RC     AT  43
CONNECT IS X3  RC AT   8
CONNECT IS E2  RC AT  15
CONNECT IS E1  RC AT  16
CONNECT IS X3  RC AT  35
CONNECT IS E1  RC AT  45
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  44

STEREO ATTRIBUTES: NONE
L7          242 SEA FILE=REGISTRY SSS FUL L4.

100.0% PROCESSED  366449 ITERATIONS                     242 ANSWERS
SEARCH TIME: 00.00.04


     (FILE 'HOME' ENTERED AT 10:44:06 ON 12 MAR 2007)
```

SEARCH HISTORY

```
FILE 'REGISTRY' ENTERED AT 10:44:32 ON 12 MAR 2007
                D SAVED
                ACT BER645FULL/A
               ---------
L1              STR
L2       258797 SEA SSS FUL L1
               ---------
L3              STR L1
L4              STR L3
L5            1 SEA SSS SAM L4
                D SCAN
L6       366449 SEA SSS FUL L4 EXTEND
L7          242 SEA SSS FUL L4
                SAVE TEMP L7 BER537FULL/A

     FILE 'CAPLUS' ENTERED AT 11:23:54 ON 12 MAR 2007
L8          444 SEA ABB=ON  L7
L9              ANALYZE L8 1- RN HIT :     204 TERMS
                D

     FILE 'REGISTRY' ENTERED AT 11:25:35 ON 12 MAR 2007
L10           1 SEA ABB=ON  2002-59-7
L11           1 SEA ABB=ON  2487-40-3
L12           1 SEA ABB=ON  5437-25-2
L13         239 SEA ABB=ON  L7 NOT (L10 OR L11 OR L12)

     FILE 'CAPLUS' ENTERED AT 11:25:52 ON 12 MAR 2007
L14         122 SEA ABB=ON  L13
L15         410 SEA ABB=ON  L8 AND (PY<2003 OR AY<2003 OR PRY<2003)
L16         117 SEA ABB=ON  L14 AND L15

     FILE 'REGISTRY' ENTERED AT 11:26:51 ON 12 MAR 2007

     FILE 'CAPLUS' ENTERED AT 12:15:58 ON 12 MAR 2007
                E US2004-511537/APPS
L17           1 SEA ABB=ON  US2004-511537/AP
                D SCAN
                SEL RN

     FILE 'REGISTRY' ENTERED AT 12:16:34 ON 12 MAR 2007
L18          79 SEA ABB=ON  (102353-42-4/BI OR 105-56-6/BI OR 111538-46-6/BI
                OR 139460-80-3/BI OR 139460-81-4/BI OR 139460-82-5/BI OR
                1516-33-2/BI OR 263552-78-9/BI OR 37412-64-9/BI OR 405-74-3/BI
                OR 436094-96-1/BI OR 56541-07-2/BI OR 591-82-2/BI OR 59814-51-6
                /BI OR 618913-11-4/BI OR 618913-12-5/BI OR 618913-13-6/BI OR
                618913-14-7/BI OR 618913-15-8/BI OR 618913-16-9/BI OR 618913-17
                -0/BI OR 618913-18-1/BI OR 618913-19-2/BI OR 618913-20-5/BI OR
                618913-21-6/BI OR 618913-22-7/BI OR 618913-23-8/BI OR 618913-24
                -9/BI OR 618913-25-0/BI OR 618913-26-1/BI OR 618913-27-2/BI OR
                618913-28-3/BI OR 618913-29-4/BI OR 618913-30-7/BI OR 618913-31
                -8/BI OR 618913-32-9/BI OR 618913-33-0/BI OR 618913-34-1/BI OR
                618913-35-2/BI OR 618913-36-3/BI OR 618913-37-4/BI OR 618913-38
                -5/BI OR 618913-39-6/BI OR 618913-40-9/BI OR 618913-41-0/BI OR
                618913-42-1/BI OR 618913-43-2/BI OR 618913-44-3/BI OR 618913-45
                -4/BI OR 618913-46-5/BI OR 618913-47-6/BI OR 618913-48-7/BI OR
                618913-49-8/BI OR 618913-50-1/BI OR 618913-51-2/BI OR 618913-53
                -4/BI OR 618913-55-6/BI OR 618913-56-7/BI OR 618913-57-8/BI OR
                618913-58-9/BI OR 618913-59-0/BI OR 618913-60-3/BI OR 618913-61
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                -4/BI OR 618913-62-5/BI OR 618913-63-6/BI OR 618913-64-7/BI OR
                618913-65-8/BI OR 618913-66-9/BI OR 618913-67-0/BI OR 618913-68
                -1/BI OR 63908-28-1/BI OR 66892-25-9/BI OR 66892-28-2/BI OR
                66892-33-9/BI OR 6815-00-5/BI OR 75914-95-3/BI OR 75914-97-5/BI
                 OR 81250-28-4/BI OR 9003-99-0/BI)
                D SCAN
                E MYELOPEROXIDASE/CN
L19           1 SEA ABB=ON  MYELOPEROXIDASE/CN

     FILE 'REGISTRY' ENTERED AT 12:30:15 ON 12 MAR 2007
                D IDE

     FILE 'CAPLUS' ENTERED AT 12:31:34 ON 12 MAR 2007
L20           1 SEA ABB=ON  L17 AND L8

     FILE 'CAPLUS' ENTERED AT 12:31:52 ON 12 MAR 2007
                D IBIB ED ABS HITSTR
L21       42778 SEA ABB=ON  L19
L22           1 SEA ABB=ON  L21 AND L8
                D SCAN
L23        4978 SEA ABB=ON  NEUROINFLAM?/OBI OR (NERV?/OBI OR NEURON?/OBI)(L)IN
                FLAM?/OBI
L24           1 SEA ABB=ON  L23 AND L8

     FILE 'REGISTRY' ENTERED AT 12:34:15 ON 12 MAR 2007
                D QUE L7
L25             STR L4
L26          13 SEA SUB=L7 SSS SAM L25
                D QUE NOS
L27             STR L4
                D SCAN L10
                D SCAN L11
                D SCAN L12
L28          22 SEA ABB=ON  L7 AND L18
L29          22 SEA ABB=ON  L28 NOT (L10 OR L11 OR L12)

     FILE 'CAPLUS' ENTERED AT 14:17:20 ON 12 MAR 2007
L30           2 SEA ABB=ON  L29

     FILE 'REGISTRY' ENTERED AT 14:17:55 ON 12 MAR 2007
                D SCAN L29

     FILE 'STNGUIDE' ENTERED AT 14:18:07 ON 12 MAR 2007

     FILE 'REGISTRY' ENTERED AT 14:25:23 ON 12 MAR 2007
L31          21 SEA ABB=ON  L7 AND CHOLINE
                D SCAN

     FILE 'CAPLUS' ENTERED AT 14:27:08 ON 12 MAR 2007
L32           3 SEA ABB=ON  L31

     FILE 'STNGUIDE' ENTERED AT 14:27:23 ON 12 MAR 2007

     FILE 'CAPLUS' ENTERED AT 14:35:51 ON 12 MAR 2007
                D SCAN L17
L33          48 SEA ABB=ON  L8(L)(THU OR PAC OR BAC OR PKT OR DMA)/RL
L34     2186237 SEA ABB=ON  PHARMAC?/SC,SX
L35         145 SEA ABB=ON  L8 AND L34
L36          43 SEA ABB=ON  L35 AND L14
L37          80 SEA ABB=ON  L33 OR L36
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     FILE 'REGISTRY' ENTERED AT 14:39:47 ON 12 MAR 2007
L38            1 SEA ABB=ON  2398-70-1
L39          238 SEA ABB=ON  L13 NOT L38

     FILE 'CAPLUS' ENTERED AT 14:40:05 ON 12 MAR 2007
L40          109 SEA ABB=ON  L39

     FILE 'STNGUIDE' ENTERED AT 14:41:29 ON 12 MAR 2007
     FILE 'REGISTRY' ENTERED AT 14:42:39 ON 12 MAR 2007
                D STAT QUE L8
                D IDE L10

     FILE 'CAPLUS' ENTERED AT 14:44:19 ON 12 MAR 2007
L41          192 SEA ABB=ON  L10
L42          122 SEA ABB=ON  L41 NOT ((L11 OR L12 OR L13))
L43           24 SEA ABB=ON  L42 AND P/DT
                D IBIB ED ABS HITSTR 20-24

     FILE 'REGISTRY' ENTERED AT 14:46:08 ON 12 MAR 2007
                D IDE L11

     FILE 'CAPLUS' ENTERED AT 14:46:16 ON 12 MAR 2007
L44          154 SEA ABB=ON  L11
L45           89 SEA ABB=ON  L44 NOT ((L12 OR L10 OR L13))
L46           52 SEA ABB=ON  L45 AND P/DT
                D IBIB ED ABS HITSTR 48-52

     FILE 'REGISTRY' ENTERED AT 14:47:20 ON 12 MAR 2007
                D IDE L12

     FILE 'CAPLUS' ENTERED AT 14:47:27 ON 12 MAR 2007
L47           48 SEA ABB=ON  L12 NOT ((L10 OR L11 OR L13))
L48           16 SEA ABB=ON  L47 AND P/DT
                D IBIB ED ABS HITSTR 12-16

     FILE 'REGISTRY' ENTERED AT 14:48:47 ON 12 MAR 2007
                D QUE NOS L7
L49             STR L4
L50           14 SEA SUB=L7 SSS SAM L49
L51             STR L49
L52           13 SEA SUB=L7 SSS SAM L51
                D SCAN
L53          242 SEA SUB=L7 SSS FUL L51 EXTEND
L54          212 SEA SUB=L7 SSS FUL L51
                SAVE TEMP L54 BER537SUB1/A
L55          209 SEA ABB=ON  L54 NOT (L10 OR L11 OR L12)

     FILE 'CAPLUS' ENTERED AT 15:00:14 ON 12 MAR 2007
L56          119 SEA ABB=ON  L55
                D QUE NOS L16
     FILE 'REGISTRY' ENTERED AT 15:02:06 ON 12 MAR 2007
                D STAT QUE L7
     FILE 'CAPLUS' ENTERED AT 15:02:06 ON 12 MAR 2007
                D QUE NOS L16
L57          116 SEA ABB=ON  L16 NOT L17
                D IBIB ED ABS HITSTR 1-116

     FILE 'HOME' ENTERED AT 15:03:12 ON 12 MAR 2007
                D STAT QUE L7
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thione (IV), and 3-methyl-6-methylthiopurine (V) had C:N bonds fixed in the 1,2-position. This bond fixation alone was inadequate in explaining the rate of attack of these compds. by milk xanthine oxidase. 3-Methylxanthine (3 g.) was refluxed 2 hrs. with 15 g. P2S5 in 150 ml. C5H5N, the solvent evaporated, the residue heated with water (15 min.), and the pH brought to 9 with NH4OH. After 30 min., this solution was filtered, and the filtrate concentrated in vacuo to 50 ml. and acidified to pH 5.5 to precipitate 2.2 g. 2-hydroxy-3-methylpurine-6-thione (VI), which was purified by treatment with C in 5% NaOH, precipitated with HOAc, and recrystd. from water as yellow needles, decomposing above 300°. VI (1.2 g.) in 25 ml. N NaOH was refluxed 2 hrs. with 4 g. Raney Ni (VII), VII removed, and the solution evaporated to dryness. The residue was dissolved in 5% ethanolic H2SO4 and water added to just clarify the solution which, after treatment with C and storage at 0°, deposited 23% 3-methyl-2-purinone (VIII) as the sulfate in large colorless plates. VIII, colorless needles, decomposed 297-300° (EtOH). Similarly, 0.2 g. 3-methyl-6-thiouric acid refluxed 70 min. with 0.8 g. VII in 20 ml. 5% NH4OH gave, on acidification and cooling, 90 mg. 8-hydroxy-3-methyl-2- purinone, flat rods, decomposing above 300° (water). 1,2-Dihydro-1-methyl-2-thio-4-hydroxy-5,6-diaminopyrimidine (IX) (CA 55, 2656g) (3.3 g.) and 12 ml. HCONH2 heated 1.5 hrs. at 180-90° gave, on cooling, 3.2 g. 6-hydroxy-3-methylpurine-2-thione (X), prisms, decomposing above 300° (water). X (3 g.) was heated to 90° in 70 ml. 5% NH4OH, 9 g. VII added, and heating and stirring continued 2 hrs. to give, on cooling and concentration of the solution, 1.9 g. I, colorless needles, decomposing above 300° (50% EtOH) (crystallizing with 1/3 H2O). Heating 1 g. IX and 1 g. CO(NH2)2 20 min. at 195°, dissolving the product in 5% NaOH, treating with C, and acidifying with 20% H2SO4pptd. 90% 6,8-dihydroxy-3-methylpurine-2-thione (XI), decomposing above 300°. Desulfurization of XI in 10 ml. N NaOH (refluxed 1.5 hrs. with 1.5 g. VII) followed by acidification with 20% H2SO4 gave 0.3 g. II, colorless plates, decomposing above 300° (H2O). 2,6-Dimercapto-3-methyl-8-purinol (1 g.) in 10 ml. 2.5% NaOH was refluxed with stirring with 2 g. VII; after 45 min., 2 g. VII was added and refluxing continued 70 min. The filtrate was brought to pH 7.5 with HOAc, evaporated to dryness, and the residue extracted with cold EtOH. The residue was crystallized from hot 90% EtOH to give 250 mg. III, subliming about 250°, m. above 300°. Treatment of 0.8 g. XI with 2.5 g. P2S5 in 45 ml. C5H5N (as in the preparation of VI) gave 68% 2-mercapto-3-methylpurine-6-thione (XII), yellowish elongated prisms, decomposing above 300° (Me2NCHO-water). Refluxing 1.1 g. I with 5 g. P2S5 in 60 ml. C5H5N 4 hrs. gave, after evaporation of solvent and treatment with hot water, 0.8 g. IV, yellowish pointed prisms, decomposing above 300° (H2O). Treatment of 0.4 g. IV in 5 ml. 2.5% NaOH at room temperature with 0.3 ml. MeI (2 hrs.) gave 0.4 g. V, colorless prisms (water), m. 166°. IV, V, and XII could not be desulfurized to 3-methylpurine.

IT **28139-02-8P**, Xanthine, 3-methyl-2-thio- **33285-76-6P**, Xanthine, 3-methyl-6-thio-
RL: PREP (Preparation)
(preparation of)

RN 28139-02-8 CAPLUS

CN 6H-Purin-6-one, 1,2,3,7-tetrahydro-3-methyl-2-thioxo- (9CI) (CA INDEX NAME)